



Institut für Festkörperforschung

Dynamics of Fracture and Segregation

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Dynamik der Rißbildung und Segregation

Zusammenfassung

Elastische Effekte spielen bei Phasenumwandlungen eine wichtige Rolle, wenn zumindest eine feste Phase beteiligt ist. Komplizierte Vorgänge bei der Unterkühlung oder dem Aufschmelzen mehrkomponentiger Legierungen können große elastische Verspannungen aufgrund der Dichtedifferenzen der beteiligten Komponenten hervorrufen. Bei Segregationsprozessen von Schmelzeinschlüssen innerhalb eines überhitzten Festkörpers treten starke elastische Wechselwirkungen auf und beeinflussen entscheidend das Skalenverhalten des Vergrößerungsprozesses. Ein herkömmliches Molekularfeldverhalten bricht zusammen und mehrere unabhängige Längenskalen sind zu berücksichtigen. Das Skalenverhalten für die Vergrößerung in einer Anordnung aus parallelen Einschlüssen wird hergeleitet.

Ein eng verwandtes Problem ist das Rißwachstum in einem uniaxial gespannten Festkörper. Zahlreiche Risse können in der Probe entstehen und zur Relaxation der Spannung führen; derartige Situationen können häufig in geologischen Systemen beobachtet werden. Ein starkes Wechselspiel benachbarter Risse läßt die längeren Risse auf Kosten der kürzeren wachsen.

Die Ausbreitung von Rissen zeigt einige Eigentümlichkeiten für höhere Wachstumsgeschwindigkeiten. Eine Kontinuumstheorie, die schnelles Rißwachstum durch Oberflächendiffusion beschreibt, wird vorgestellt. Durch die Einführung der vollen dynamischen Elastizitätstheorie gelingt die selbstkonsistente Selektion des Rißspitzenradius. Diese Theorie beschreibt die komplizierte Dynamik einer Rißspitze, die Sättigung der stationären Ausbreitungsgeschwindigkeit auf Werte deutlich unterhalb der Rayleighgeschwindigkeit und das Abstumpfen der Rißspitze. Desweiteren enthält sie die Möglichkeit einer Spitzenverzweigungsinstabilität für hohe Zugspannungen.

Dynamics of Fracture and Segregation

Abstract

Elastic effects play an important role in phase transitions if at least one solid phase is involved. Complicated processes during the undercooling or melting of multi-component alloys can produce high elastic stresses due to differences in the densities of the involved ingredients. During the segregation of melt inclusions inside an overheated solid, strong elastic interactions can appear and significantly modify the scaling behavior of the coarsening process. The usual mean-field behavior breaks down and several independent length scales have to be taken into account. The scaling laws for the coarsening in a system of parallel inclusions are derived.

A closely related problem is the growth of cracks in a uniaxially strained solid. Several cracks can appear in the sample and lead to a relaxation of stresses; situations like this can often be observed in geological systems. A strong interplay between neighboring cracks lets the longer cracks grow at the expense of the shorter ones.

Crack propagation exhibits several peculiarities for higher propagation velocities. A continuum theory which describes the fast growth of a crack by surface diffusion is presented. By introducing a fully dynamical theory of elasticity, it is possible to produce a self-consistent selection of the crack tip radius. This theory describes the complicated dynamics of a crack tip, the saturation of the steady state velocity appreciably below the Rayleigh speed, and the blunting of the crack tip. Furthermore, it includes the possibility of a tip splitting instability for high applied tensions.

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Chapter 1

Overview

It is hard to imagine our world without the various manifestations of elastic effects. Fracture, for example, is an intriguing irreversible phenomenon that plays an important role in our day-to-day-life. Cracks occur on all scales from nano- to kilometers: we observe them in geological formations and earthquakes, semiconductor-metal-contacts, airplane wings and buildings. They are responsible for the vast field of material failure and also for friction processes: slip motion between different solids can be interpreted as a traveling of self-healing cracks along the contact area of the interface. Complicated patterns of crack networks appear in drying mud. But even the growth of a single crack exhibits surprising features: Under some circumstances cracks propagate in a straight way, in other situations they produce rough surfaces or split to intertwined structures like in a shattered window. What is responsible for these effects? How does a crack grow? How fast can a crack move?

Obviously many complicated physical effects contribute to the observed peculiarities: Brittle-to-ductile transitions in regions around the crack tip with strong plastic flow, the emergence and motion of dislocations, granular and heterogeneous effects of the materials and also the lattice structure and bond breaking. However, this usually leads to very complicated descriptions which are based on theories which are not yet fully developed and contain many guesses.

On the other hand, experiments and everyday observations show that many of the mentioned puzzling phenomena can occur in rather different materials on different scales. This gives raise to the question whether they can possibly be explained in a *generic* way using only simple and well established theoretical concepts.

Novel aspects appear in systems of many interacting cracks with strong interactions. Microcracks are created in aging materials, grow and finally destroy the sample. Closely connected, segregation leads to inhomogeneities in a solid producing elastic stresses and possibly crack formation. It is very important to understand these processes which cause material failure in many technological applications. Therefore the question arises how the transition to the state of the fractured solid occurs.

Another important example for elastic nonequilibrium effects is the so called Asaro-Tiller-Grinfeld instability. A solid material which is subjected to an external nonhydrostatic loading is morphologically unstable; this leads to irreversible transformations at its surface. It is quite remarkable that the only condition for the occurrence of this instability, the presence of nonhydrostatic stresses, is very common in our world: Gravity leads to exactly this kind of uniaxial stress; therefore all buildings suffer from the Grinfeld instability. But why do we not

observe this effect? Why does it not lead to deformations of houses and bridges? The answer is that the underlying surface diffusion process is usually very slow. Surprisingly enough, it can become extremely fast once the instability has developed, and then it can become compatible to fracture. This becomes evident in heteroepitaxial growth of semiconductors where the Grinfeld instability can be responsible for island formation on substrates; this can be used for creation of quantum dots. Recently, the idea was developed that the fast evolution of this instability can lead to important effects in metallurgical melting-recrystallization processes. Possibly, use can be made of the strong influence of elastic effects for the design of new composite materials.

In fact, both crack propagation and Grinfeld instability arise due to a competition between a decrease of elastic energy and an increase of surface energy. It is one aim of this thesis to elucidate similarities of these effects and to demonstrate that they are even more closely related. This already shows that elastic effects are not only relevant on all lengthscales, but also on very different timescales - from fast crack growth to the alleged Asaro-Tiller-Grinfeld instability.

Elastic effects also play an important role in phase transitions if at least one solid phase is involved. Complicated processes during the undercooling or melting of multi-component alloys can produce high elastic stresses due to concentration profiles, temperature gradients and differences in the densities of the involved ingredients. During the segregation of melt inclusions inside an overheated solid, strong elastic interactions can appear and significantly modify the scaling behavior of the coarsening process. At a first glance, this seems to be a subject which is far away from fracture mechanics. Although the fundamentals of first order phase transitions and also the basic principles of crack propagation are separately known already for a long time, only recently the interconnecting interpretation of the emergence of cracks as a nucleation process was given. We emphasize new links between both fields of research in this thesis. In fact, the Grinfeld instability is one of the main connections, and combination of these separate ideas can lead to new insights.

This thesis is organized as follows:

Chapter 2 starts with an overview about the conventional linear theory of elasticity and presents the basic notations. A brief introduction to the fundamental principles of fracture mechanics is given, discussing the necessity of a fully dynamical theory. This chapter also reviews the Asaro-Tiller-Grinfeld instability of a uniaxially strained elastic body.

The first results are given in **chapter 3**. We discuss the influence of surface tension on the Grinfeld instability. This requires the derivation of the governing equations from a fundamental variational principle. Here we establish a consistent way to derive the driving forces and exact boundary conditions.

In **chapter 4** we study the coarsening of a melt phase in an overheated crystalline matrix. We explain why the standard mean field behavior must break down, how several relevant lengthscales enter into the system and how the scaling laws are changed in comparison to the “classical” situation without long-range elastic and thermal interactions. This situation is rather complicated due to a strong interplay between neighboring inclusions, and it is quite astonishing that nevertheless analytical scaling laws can be derived in a system of melt inclusions. These precipitates exhibit a crack-like shape and many parallels can be drawn to fracture processes.

These similarities are extended in **chapter 5**. Here we analyze how cracks develop in a strained solid; situations like this can often be observed in geological systems, especially in

earthquakes. The appearance of cracks lead to a relaxation of stresses and to complicated interactions between neighboring cracks. In the coarsening regime, this scenario is very much comparable to the late stage of a first order phase transition: Larger cracks can grow at the expense of smaller ones which can even reheal and disappear under certain circumstances. Dynamics lead to stress relaxation, and finally the sample is torn into pieces. We derive the scaling laws of the coarsening process which describe in a robust way the transition to the equilibrium state.

In **chapter 6** we look in more detail at the growth of a single crack and study the dynamical processes in the tip region. We present the concept of crack growth by diffusion along the surfaces of the crack. Based only on a few well-established ingredients, surface diffusion and the linear theory of elasticity, we can describe self-consistently fast crack propagation, velocity limitations and even a tip-splitting instability. We clear up the long-standing puzzle of an unphysical cusp singularity in the Grinfeld instability and relate this subject to the field of fracture mechanics. Introducing a local stress model, we derive the propagation velocity, the tip radius and the shape of a crack as functions of the applied force.

Chapter 7 continues the preceding chapter by providing the tools to solve the full problem of crack growth by surface diffusion. We go beyond the simplifications of the local model and derive all exact equations in the framework of this concept of fracture mechanics. We present the developed numerical tools together with some applications to check their consistency and to confirm former results. They are applied to the problem of growth of a melt finger in a channel, which is related to the crack growth by surface diffusion again via the Grinfeld instability. Effectively, it describes details of the growth of a melt inclusion inside a solid phase, and we have come full circle to chapter 4.

In **chapter 8** a short summary of the results of this thesis is given.

Chapter 2

Introduction

In this chapter we give an introduction to specific subjects involving elastic effects, which are of high relevance for the successive parts of this thesis.

In sections 2.1 to 2.3 basic notations and a brief presentation of the main relations of the static theory of elasticity are given.

Section 2.4 introduces a very important concept of the theory of cracks, the so called *Griffith condition*. The energetic scaling arguments deduced there are relevant for many fracture processes. In section 2.5 an exact solution of the elastic problem of a semi-infinite crack in a two-dimensional solid is given. We derive the singular behavior of stresses in the vicinity of the crack tip. This property is very generic and related to the so-called *stress intensity factor* which is explained in section 2.6.

A completely different subject, the *Asaro-Tiller-Grinfeld instability*, is presented in section 2.8. It states that a solid with a nonhydrostatic stress state at its surface suffers from an instability due to morphological rearrangements of matter along its surface. In the following chapters, in particular in chapter 6, it will be shown that this phenomenon is closely related to fracture mechanics.

Finally, in section 2.9, a concise introduction to the theory of bending of thin plates is given. This will be required to understand the coarsening of a melt phase in a superheated solid (chapter 4) and the collective growth of cracks in a uniaxially strained solid (chapter 5).

2.1 The linear theory of elasticity

We assume that all quantities are given in a fixed, orthonormal frame of reference. The coordinates of all points of the undisplaced body are given by a vector field x_i . External forces deform the body, and the mass points move to new coordinates $x_i^*(\{x_j\})$, which are functions of the original coordinates. The quantity

$$u_i(\{x_j\}) = x_i^*(\{x_j\}) - x_i \quad (2.1)$$

is called *displacement vector* and is assumed to be small. The *strain field* is defined as

$$u_{ij} = \frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right), \quad (2.2)$$

which is a symmetric tensor.

σ_{ij} denotes the *stress field*. Its physical meaning is that its component i gives the elastic force density per unit area which acts on a plane with normal $\mathbf{e}_j$. The conservation of angular momentum implies the symmetry of σ_{ij} [54]. In the linear theory of elasticity the connection between stresses and strain is given by *Hooke's law*; we need it only for the special case of isotropic materials:

$$\sigma_{ij} = \frac{E}{1+\nu} \left(u_{ij} + \frac{\nu}{1-2\nu} \delta_{ij} u_{kk} \right), \quad (2.3)$$

with E being the elastic modulus and ν the Poisson ratio. The inverse transformation is

$$u_{ij} = \frac{1}{E} [(1+\nu)\sigma_{ij} - \nu\delta_{ij}\sigma_{kk}]. \quad (2.4)$$

Newton's equation of motion reads

$$\frac{\partial \sigma_{ij}}{\partial x_i} + F_j = \rho \ddot{u}_i, \quad (2.5)$$

with a density F_j of volume forces and the mass density ρ . In many cases, the right hand side can be neglected.

Quite often one discusses elastic problems on the level of strains and stresses instead of displacement. However, it has to be assured that they can be derived from the latter ones. The necessary integration condition is called *St. Venant's compatibility condition*:

$$\frac{\partial^2 u_{ij}}{\partial x_k \partial x_l} + \frac{\partial^2 u_{kl}}{\partial x_i \partial x_j} = \frac{\partial^2 u_{ik}}{\partial x_j \partial x_l} + \frac{\partial^2 u_{jl}}{\partial x_i \partial x_k}. \quad (2.6)$$

2.2 Plane strain

The body is in a state of *plane strain* parallel to the xy plane if the displacement component u_z vanished, $u_z = 0$, and u_x, u_y depend only on x and y . Thus

$$\sigma_{xz} = \sigma_{zx} = 0, \quad \sigma_{yz} = \sigma_{zy} = 0, \quad (2.7)$$

and

$$\sigma_{zz} = \lambda(u_{xx} + u_{yy}), \quad (2.8)$$

with $\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$.

We assume that no body forces are present in (2.5) and that we can refrain from the inertial terms. Then the equilibrium equations are equivalent to the derivability of the stresses from an *Airy function* $U(x, y)$ [42]

$$\sigma_{xx} = \frac{\partial^2 U}{\partial y^2}, \quad \sigma_{xy} = -\frac{\partial^2 U}{\partial x \partial y}, \quad \sigma_{yy} = \frac{\partial^2 U}{\partial x^2}. \quad (2.9)$$

Compatibility (2.6) is equivalent to the biharmonic equation

$$\Delta \Delta U = 0 \quad \text{or} \quad \frac{\partial^4 U}{\partial x^4} + 2 \frac{\partial^4 U}{\partial x^2 \partial y^2} + \frac{\partial^4 U}{\partial y^4} = 0. \quad (2.10)$$

2.3 Complex representation

For the two-dimensional, static plane-strain situation the application of complex analysis turns out to be useful. We write $z = x + iy$. A complex function $\varphi(z) = f(x, y) + ig(x, y)$ is analytic if and only if the Cauchy-Riemann equations are fulfilled:

$$\frac{\partial f}{\partial x} = \frac{\partial g}{\partial y}, \quad \frac{\partial f}{\partial y} = -\frac{\partial g}{\partial x}. \quad (2.11)$$

An Airy function which obeys the biharmonic equation (2.10) can be constructed as [54]

$$U(x, y) = \Re(\bar{z}\varphi(z) + \chi(z)), \quad (2.12)$$

where $\varphi(z)$ and $\chi(z)$ are two arbitrary analytic functions. Stresses can be derived from

$$\sigma_{xx} + \sigma_{yy} = 4\Re(\varphi'(z)), \quad (2.13)$$

$$\sigma_{yy} - \sigma_{xx} + 2i\sigma_{xy} = 2(\bar{z}\varphi''(z) + \chi''(z)). \quad (2.14)$$

2.4 The Griffith criterion

The basic idea about the energetics of crack formation was brought up by Griffith [33]: Consider an infinite two-dimensional solid which is subjected to an external tension P (see Fig. 2.1). For simplicity, the material is assumed to be homogeneous and isotropic, and

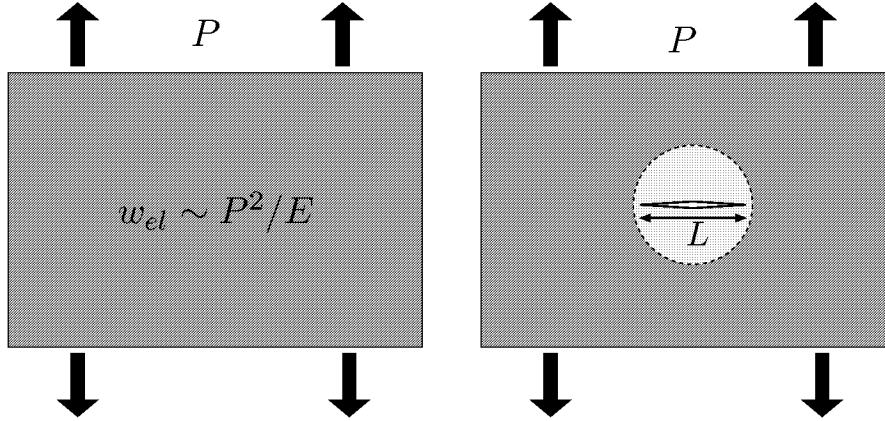


Figure 2.1: An initially homogeneously stretched body reduces its elastic energy by producing a crack. On the other hand, this increases the surface energy of the system.

the static linear theory of elasticity is used. In this solid, the elastic energy density is¹ $w_{el} \sim P^2/E$, where E is the elastic modulus. We compare this situation to a solid which contains a finite crack of length L . Approximately, in the area $A \sim L^2$ the initial stress has relaxed by the opening of the crack. Therefore, we have a total decrease of the elastic energy by $W_{el} \sim w_{el}A \sim P^2L^2/E$. On the other hand, we produced the new crack surfaces which increase the surface energy of the system by $W_s \sim \alpha L$, with α being the surface energy

¹The dimensionless Poisson ratio is of order unity and does not alter the scaling behavior. We suppress it here.

density. The total energy $W = W_{el} + W_s$ is therefore bigger than the total energy of the undestroyed solid for short cracks, but becomes smaller for sufficiently long cracks (see Fig. 2.2). In fact, the stretched solid is far from equilibrium where it is completely broken into

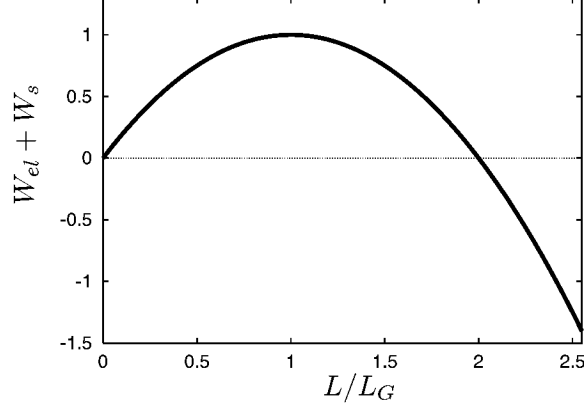


Figure 2.2: The total energy of the system has a maximum at the Griffith length.

pieces. The critical length

$$L_G \sim \frac{E\alpha}{P^2} \quad (2.15)$$

is called the Griffith length of the crack and determines the metastable length of the crack which maximizes the total energy. The exact value of the Griffith length also depends on the shape of the crack.

Assuming the simplest linear response law for extension of the crack

$$\dot{L} = -\gamma \frac{dW}{dL} \quad (2.16)$$

with a kinetic coefficient γ immediately shows a serious problem: In the infinite solid the crack accelerates further and further and reaches an infinite velocity after a finite time. The static linear theory of elasticity does not provide a cutoff mechanism for propagation velocities. Furthermore, a steady state growth with constant velocity is not possible in this configuration for fixed external loading.

This problem can easily be cured in a strip geometry which is mostly used in experiments. Here a fixed external displacement $u_y^{(ext)}$ is applied to the strip, perpendicular to the propagation direction of the crack (see Fig 2.3). The initial homogeneous energy density is $w_{el} \sim Eu_y^{(ext)2}/B^2$. The relaxed area is $A \sim LB$, where we assume the crack length L to be much bigger than the strip width, $L \gg B$. Therefore, the total decrease of elastic energy is $W_{el} \sim -Eu_y^{(ext)2}L/B$. Far away from the tip at distances $L \gg r \gg B$, the opening of the crack has reached the value $u_y^{(ext)}$; the elastic body is completely relaxed there. The surface energy is $W_s \sim \alpha L$. Crack growth or shrinkage according to (2.16) is now completely determined by the strength of the external tension and does not depend on the length of the crack [26]:

$$u_y^{(ext,crit)} \sim \left(\frac{B\alpha}{E} \right)^{1/2} \quad (2.17)$$

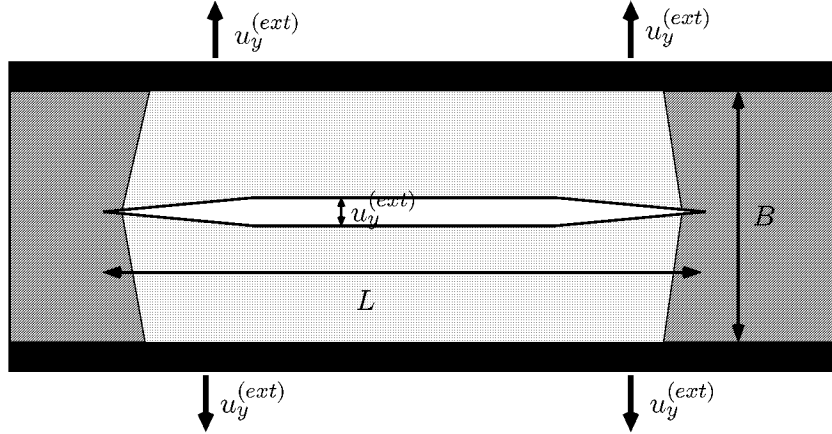


Figure 2.3: A strip of width B is subjected to a fixed external displacement $u_y^{(ext)}$. In the region where a crack appears, the material is completely relaxed.

From $W \sim W_{el} + W_s \sim L(-Eu^{(ext)2}/B + \alpha)$ follows readily that the dissipation rate dW/dL is independent of L ; this resolves the impossibility of a steady state growth with fixed external loading.

One can also study the strip problem with given external *tension*. In this case the opening increases with increasing distance from the tip. This problem is related to the bending of thin plates (see section 2.9).

2.5 The static semi-infinite crack

In this section we derive the elastic fields for an infinite solid which contains a semi-infinite straight crack (see Fig. 2.4). In particular, we are interested in the divergent part of the stresses in the vicinity of the infinitely sharp crack tip.

We consider a two-dimensional, plane strain material. We make the separation ansatz for the Airy function (2.9)

$$U = Ar^m e^{in\theta} \quad (2.18)$$

in polar coordinates; n and m are arbitrary real numbers. Real and imaginary parts are intended to be independent solutions.

Since in polar coordinates

$$\Delta = \frac{\partial^2}{\partial r^2} + \frac{1}{r^2} \frac{\partial}{\partial \theta^2} + \frac{1}{r} \frac{\partial}{\partial r}, \quad (2.19)$$

we obtain

$$\Delta \Delta U = Ae^{in\theta} r^{m-4} (m^2 - n^2) ((m-2)^2 - n^2). \quad (2.20)$$

Thus we get 4 independent real solutions of the fourth order equation (2.10) with either $n = m$ or $n = m - 2$

$$U^{(1)} = r^m \cos m\theta, \quad (2.21)$$

$$U^{(2)} = r^m \sin m\theta, \quad (2.22)$$

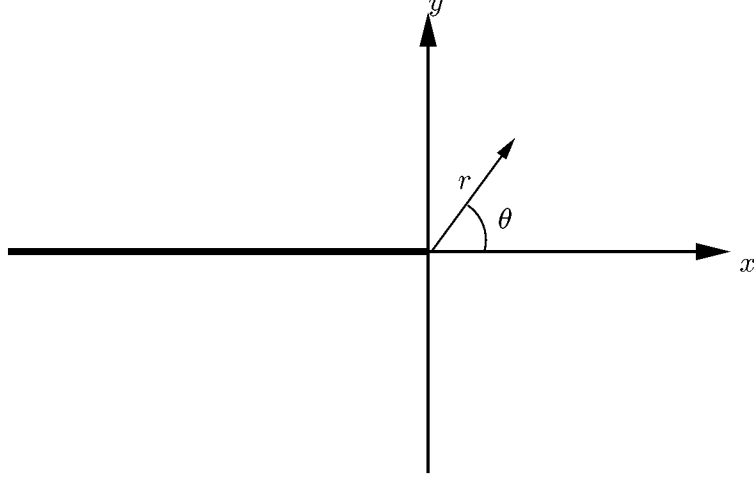


Figure 2.4: Semi-infinite crack along the negative real axis.

$$U^{(3)} = r^m \cos(m-2)\theta, \quad (2.23)$$

$$U^{(4)} = r^m \sin(m-2)\theta. \quad (2.24)$$

In particular, we are interested in a crack geometry, which is given by the mathematical cut along the negative x axis (see Fig. 2.4). We study only the singular solution with $m < 0$. They exhibit the characteristic singularity of stresses at the crack tip.

The spatial derivatives are

$$\left(\frac{\partial}{\partial x}\right)_y = \cos\theta \left(\frac{\partial}{\partial r}\right)_\theta - \frac{\sin\theta}{r} \left(\frac{\partial}{\partial \theta}\right)_r \quad (2.25)$$

$$\left(\frac{\partial}{\partial y}\right)_x = \sin\theta \left(\frac{\partial}{\partial r}\right)_\theta + \frac{\cos\theta}{r} \left(\frac{\partial}{\partial \theta}\right)_r \quad (2.26)$$

The so called *mode I of loading* (see also section 2.6) with an external force perpendicular to the crack plane forbids by symmetry the fundamental solutions containing $\sin$, therefore only the two independent solutions (2.21) and (2.23) remain. The general solution is thus a linear combination of $U^{(1)}$ and $U^{(3)}$. They lead to stress components according to Eqs. (2.9)

$$\sigma_{xx}^{(1)} = -r^{m-2}m(m-1)\cos(m-2)\theta \quad (2.27)$$

$$\sigma_{xx}^{(2)} = r^{m-2} \left((-m^2 + 3m - 2)\cos(m-4)\theta + 2(m-1)\cos(m-2)\theta \right) \quad (2.28)$$

$$\sigma_{xy}^{(1)} = r^{m-2}m(m-1)\sin(m-2)\theta \quad (2.29)$$

$$\sigma_{xy}^{(2)} = r^{m-2}(m^2 - 3m + 2)\sin(m-4)\theta \quad (2.30)$$

$$\sigma_{yy}^{(1)} = r^{m-2}m(m-1)\cos(m-2)\theta \quad (2.31)$$

$$\sigma_{yy}^{(2)} = r^{m-2} \left((m^2 - 3m + 2)\cos(m-4)\theta + 2(m-1)\cos(m-2)\theta \right) \quad (2.32)$$

where the superscript 1 corresponds to $n = m$ and 2 to $n = m - 2$.

Boundary conditions require that the normal and shear components of the total stress

$$\sigma_{ij} = A_1\sigma_{ij}^{(1)} + A_2\sigma_{ij}^{(2)} \quad (2.33)$$

vanish on the cut $x < 0, y = 0$ or $\theta = \pm\pi$ for properly chosen weight factors A_1 and A_2 . The determinant solvability condition

$$\det \begin{pmatrix} \sigma_{yy}^{(1)}(\theta = \pi) & \sigma_{yy}^{(2)}(\theta = \pi) \\ \sigma_{xy}^{(1)}(\theta = \pi) & \sigma_{xy}^{(2)}(\theta = \pi) \end{pmatrix} = 0 \quad (2.34)$$

leads to the equation

$$-r^{2m-4}m \sin(2m\pi)(m-1)^2 = 0. \quad (2.35)$$

Possible solutions are

$$m = 0, \quad m = 1, \quad m = 0, \pm\frac{1}{2}, \pm 1, \pm\frac{3}{2}, \pm 2, \dots \quad (2.36)$$

We are currently interested in solutions with finite energy in the tip region, i.e. $\sigma^2 r < \infty$ for $r \rightarrow 0$. Consequently, we demand $m \geq 3/2$. On the other hand, we demand singular contributions with $\sigma \rightarrow \infty$ for $r \rightarrow 0$, which imposes $m < 2$. Thus only $m = 3/2$ remains; it leads to the well-known $r^{1/2}$ -singularity of the stresses. The solution is $A_1 = A_2/3 = K_I/(2\pi)^{1/2}$, where we introduced the mode I stress intensity factor K_I . The meaning of this scalar quantity is studied in more detail in section 2.6. We finally obtain

$$\begin{pmatrix} \sigma_{xx} \\ \sigma_{xy} \\ \sigma_{yy} \end{pmatrix} = \frac{K_I}{(2\pi r)^{1/2}} \cos(\theta/2) \begin{pmatrix} 1 - \sin(\theta/2) \sin(3\theta/2) \\ \sin(\theta/2) \cos(3\theta/2) \\ 1 + \sin(\theta/2) \sin(3\theta/2) \end{pmatrix}. \quad (2.37)$$

This is the exact solution for the singular part the stress field for a semi-infinite crack. It does not contain a homogeneous contribution which arises due to the tensile force which is applied infinitely far away. For a finite crack of length L , the preceding results are valid at distances r from the tip which are much smaller than the crack length, $r \ll L$.

2.5.1 Complex representation

We can also employ the complex representation of section 2.3. The solutions (2.21) and (2.22) with $n = m$ above correspond according to Eqs. (2.12)-(2.14) to

$$\varphi^{(1)} = 0, \quad \chi^{(1)} = z^m, \quad (2.38)$$

the solutions (2.23) and (2.24) with $n = m - 2$ to

$$\varphi^{(2)} = z^{m-1}, \quad \chi^{(2)} = 0. \quad (2.39)$$

The allowed coefficients which satisfy the boundary conditions are again those of (2.36). Notice that most of them do not correspond to functions which are analytic *everywhere* but have a jump along the negative real axis!

2.6 The near-tip behavior

The results of the previous section can be generalized to other types of cracks. In all cases we discuss two-dimensional solids, but not only plane strain situations. One of the most intriguing results for the semi-infinite crack was the characteristic $r^{-1/2}$ singularity of stresses close to the crack tip, see Eq. (2.37). Similarly, displacements behave like $r^{1/2}$.

One observes this behavior also with other cracks with a sharp tip. We distinguish between three types of loading (see Fig. 2.5),

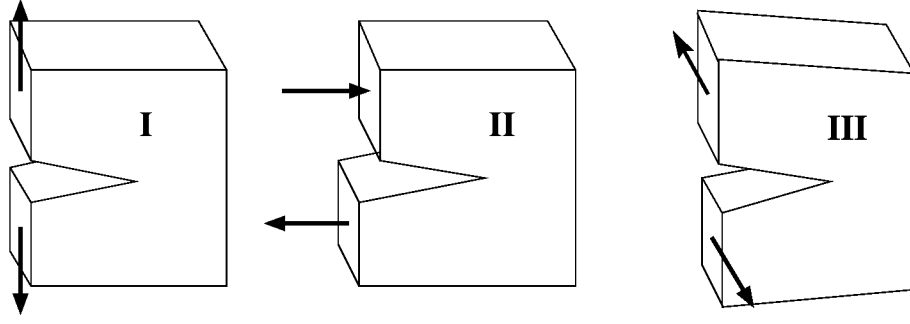


Figure 2.5: The three different types of loading near a crack tip.

- opening mode (mode *I*),
- implane sliding (mode *II*),
- antiplane sliding (mode *III*).

A general loading can always be decomposed into these three modes. In each case, stresses behaves like [59]

$$\sigma_{ij} = \frac{K}{(2\pi r)^{1/2}} f_{ij}(\theta). \quad (2.40)$$

The angular dependence $f_{ij}(\theta)$ is a universal function for each loading mode. For mode *I* it is given by Eq. (2.37). The scalar quantity K is called *stress intensity factor* and combines all the macroscopic properties of the crack including length, external forces and shape of the crack. With the characteristic external stress P and crack length L , the stress intensity factor behaves like

$$K \sim PL^{1/2}. \quad (2.41)$$

Elongation of a crack reduces the elastic energy which is stored in the system. The rate of change is given by [67]

$$-\frac{dU_{el}}{dL} = \frac{1-\nu^2}{E}(K_I^2 + K_{II}^2) + \frac{1}{2G}K_{III}^2. \quad (2.42)$$

The Griffith point is determined by the equilibrium of elastic and surface energy

$$\frac{dU_{el}}{dL} + 2\alpha = 0. \quad (2.43)$$

2.7 Dynamic fracture mechanics

2.7.1 Dimensional analysis

As we saw in section 2.4, the static theory of elasticity does not provide an upper limit for the propagation velocity of a crack. Therefore, under certain circumstances inertial effects have to be taken into account. We have to go beyond the quasistatic approximation and use the complete version of Newton's equation

$$\frac{\partial \sigma_{ij}}{\partial x_j} = \rho \ddot{u}_i, \quad (2.44)$$

with the mass density ρ . Using the results obtained above, we can estimate when this effect becomes relevant. At a distance r from a crack tip which propagates with velocity v in a certain direction, stresses behave like $\sigma_{ij} \sim Kr^{-1/2}$, and corresponding displacements $u_i \sim Kr^{1/2}/E$. The characteristic accelerations are $\ddot{u}_i \sim Kv^2r^{-3/2}/E$. Consequently, the right hand side of (2.44) becomes of the same order of magnitude as the left hand side if velocity approaches

$$v_R \sim (E/\rho)^{1/2}. \quad (2.45)$$

This relation defines the scale of the speed of sound in the material and also an upper limit for the propagation velocity for cracks.

2.7.2 Rayleigh surface waves

Whereas the static theory of elasticity allows instantaneous propagation of shocks, the inertial terms in (2.45) set an upper limit for all velocities. In particular, a sudden displacement at the interface of a solid travels with the so called *Rayleigh speed* along this surface. This velocity is a very central quantity in the theory of fracture, because it defines the upper limit for crack speeds.

We use the conventional referential description to derive the dispersion relation of surface waves [1]. The material considered here is a two-dimensional plane strain solid. We are searching for oscillations of the solid close to its interface located at $y \equiv 0$. We guess solutions of the type

$$u_x = Ae^{by} \exp[ik(x - ct)], \quad (2.46)$$

$$u_y = Be^{by} \exp[ik(x - ct)], \quad (2.47)$$

$$u_z = 0 \quad (2.48)$$

(the solid is in the half-plane $y \leq 0$). Plugging this into the equations of motion (2.44) gives the determinant solvability condition

$$\left[c_d^2 b^2 - (c_d^2 - c^2) k^2 \right] \left[c_s^2 b^2 - (c_s^2 - c^2) k^2 \right] = 0 \quad (2.49)$$

with the material velocities

$$c_s = \left(\frac{E}{2\rho(1+\nu)} \right)^{1/2}, \quad (2.50)$$

$$c_d = \left(\frac{E(1-\nu)}{\rho(1-2\nu)(1+\nu)} \right)^{1/2}, \quad (2.51)$$

the shear and dilatational velocity. Therefore, we obtain two independent roots

$$b_1 = k \left(1 - \frac{c^2}{c_d^2} \right)^{1/2}, \quad b_2 = k \left(1 - \frac{c^2}{c_s^2} \right)^{1/2}. \quad (2.52)$$

Notice that they are real if $c < c_s < c_d$. The corresponding amplitude relations (eigenvectors) are

$$\left(\frac{B}{A} \right)_1 = -\frac{b_1}{ik}, \quad \left(\frac{B}{A} \right)_2 = \frac{ik}{b_2}. \quad (2.53)$$

The general solution for the displacements is a superposition of both solutions:

$$u_x = (A_1 e^{b_1 y} + A_2 e^{b_2 y}) \exp(ik(x - ct)), \quad (2.54)$$

$$u_y = \left(-\frac{b_1}{ik} A_1 e^{b_1 y} + \frac{ik}{b_2} A_2 e^{b_2 y}\right) \exp(ik(x - ct)). \quad (2.55)$$

Now we want to fulfill the boundary conditions of vanishing normal and shear stresses at the *flat* surface $y = 0$. Therefore we demand

$$\sigma_{xy} = 0, \quad \sigma_{yy} = 0. \quad (2.56)$$

We obtain

$$2b_1 A_1 + \left(2 - \frac{c^2}{c_s^2}\right) k^2 \frac{A_2}{b_2} = 0, \quad (2.57)$$

$$\left(2 - \frac{c^2}{c_s^2}\right) A_1 + 2b_2 \frac{A_2}{b_2} = 0. \quad (2.58)$$

Nontrivial solutions of nonvanishing A_1, A_2 require therefore

$$\left(2 - \frac{c^2}{c_s^2}\right)^2 - 4 \left(1 - \frac{c^2}{c_d^2}\right)^{1/2} \left(1 - \frac{c^2}{c_s^2}\right)^{1/2} = 0. \quad (2.59)$$

Since there is no k -dependence in this equation there is also no dispersion for surface waves. This equation has exactly two roots $\pm c$ which are both real and obey $c < c_s < c_d$; it is called the *Rayleigh speed* $c = v_R$. It cannot be expressed in a closed form, but a good approximation is [27]

$$v_R \approx c_s \frac{0.862 + 1.14\nu}{1 + \nu}. \quad (2.60)$$

This sets the propagation velocity for elastic waves traveling along a free surface of a solid.

2.8 The Asaro-Tiller-Grinfeld (ATG) instability

2.8.1 Scaling analysis

The nominally flat surface of an elastically nonhydrostatically stressed body is unstable with respect to the growth of perturbations with wavelengths bigger than a critical wavelength. The maximally unstable mode depends on the manner of material transport (surface diffusion or evaporation/condensation). This phenomenon was first reported by Asaro and Tiller [4] and Grinfeld [35].

To illustrate this peculiar behavior, we estimate the energy difference between a flat and a corrugated elastic surface which is subjected to a uniaxial stress σ_0 . The material is assumed to be isotropic and two-dimensional. The flat solid has an elastic energy density $w_{el} \sim \sigma_0^2/E$, with the pre-stress $\sigma_{xx} = \sigma_0$. This stress can be either compressive or tensile. For simplicity, we discuss a body with a square wave surface morphology (see Fig. 2.6) [73]. In the cusps the body is elastically almost relaxed, and therefore the elastic energy (per cusp) is reduced by an amount $\Delta W_{el} \sim -c\lambda\sigma_0^2/E$. Notice that the new surface results from a redistribution of matter of the originally flat surface; the amount of material is conserved. Simultaneously,

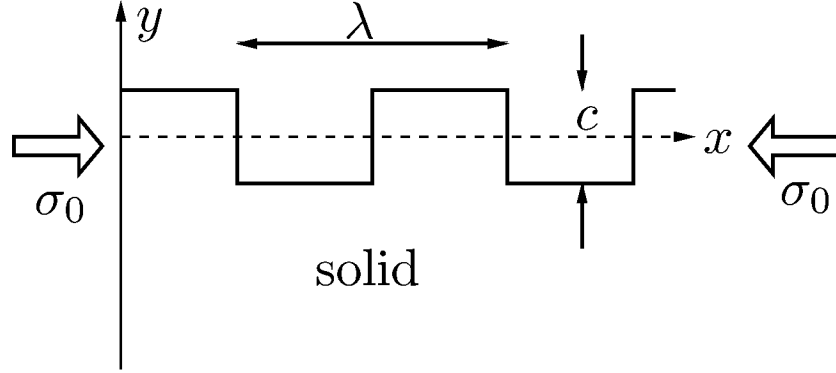


Figure 2.6: A solid with a square wave surface profile. The surface profile has wavelength λ and amplitude $c/2$. The uniaxial stress σ_0 can be either compressive or tensile; in the final expressions it appears only quadratically, therefore the sign is irrelevant.

the surface has become larger, and therefore the surface energy is increased by $\Delta W_s \sim \alpha c$. α is the surface energy density. The total change of energy is hence

$$\Delta W \sim c \left(-\frac{\sigma_0^2}{E} \lambda + \alpha \right). \quad (2.61)$$

Thus long-wave perturbations lead to a decrease of the total energy, and the solid is elastically unstable. Eq. (2.61) defines a critical wavelength

$$\lambda_c \sim \frac{\alpha E}{\sigma_0^2}. \quad (2.62)$$

Notice that this lengthscale is the same as the Griffith length. Later, it will turn out that this statement is due to a deep link between the Grinfeld instability and fracture mechanics.

2.8.2 The chemical potential

In this section we start to derive quantitative statements about the onset of the Grinfeld instability. Here we compute the driving force, the chemical potential μ at the surface, which causes a redistribution of material. In particular, for surface diffusion, the chemical potential leads to a surface flux $j \sim \nabla \mu$.

For a two-dimensional plane-strain situation we have

$$\sigma_{xz} = \sigma_{yz} = 0, \quad \sigma_{zz} = \nu(\sigma_{xx} + \sigma_{yy}). \quad (2.63)$$

Strains are

$$u_{xx} = \frac{1}{E} \left((1 - \nu^2) \sigma_{xx} - \nu(1 + \nu) \sigma_{yy} \right), \quad (2.64)$$

$$u_{yy} = \frac{1}{E} \left((1 - \nu^2) \sigma_{yy} - \nu(1 + \nu) \sigma_{xx} \right), \quad (2.65)$$

$$u_{xy} = \frac{1 + \nu}{E} \sigma_{xy}, \quad (2.66)$$

$$u_{xz} = u_{yz} = u_{zz} = 0. \quad (2.67)$$

The elastic energy density is

$$w_{el} = \frac{1}{2} \sigma_{ij} u_{ij}. \quad (2.68)$$

We choose $x = \tau$, $y = n$ and use the boundary conditions $\sigma_{nn} = \sigma_{n\tau} = 0$ at the interface. Therefore the elastic energy density at the surface is

$$w_{el} = \frac{1 - \nu^2}{2E} \sigma_{\tau\tau}^2. \quad (2.69)$$

The chemical potential is the energy density per particle. Thus

$$\mu_{el} = \Omega \frac{1 - \nu^2}{2E} \sigma_{\tau\tau}^2 \quad (2.70)$$

with the atomic volume Ω . Additionally, there is a contribution to the chemical potential from the surface energy. Variation of the arclength of the interface gives

$$\mu_s = -\Omega \alpha \kappa \quad (2.71)$$

with the surface energy density α and κ the curvature of the interface. The total chemical potential at the surface is therefore [37, 57]

$$\mu = \Omega \left(\frac{1 - \nu^2}{2E} \sigma_{\tau\tau}^2 - \alpha \kappa \right). \quad (2.72)$$

2.8.3 Interface kinetics

In this section we perform a quantitative analysis of the perturbed surface. This requires the calculation of the elastic fields for a non-flat surface profile, in order to determine the chemical potential (2.72). The physical process used here is surface diffusion. The solid phase is located below the border line

$$y(x) = \Delta \sin kx \quad (2.73)$$

(see Fig. 2.7). We assume k to be positive. We start from the Airy function (see also section 2.2)

$$U = \frac{\sigma_0 y^2}{2} + A y e^{ky} \sin kx \quad (2.74)$$

with the amplitude $A \sim \mathcal{O}(\Delta)$. Then the stresses are given by

$$\sigma_{xx} = \frac{\partial^2 U}{\partial y^2} = \sigma_0 + Ak(2 + ky)e^{ky} \sin kx, \quad (2.75)$$

$$\sigma_{yy} = \frac{\partial^2 U}{\partial x^2} = -Ak^2 y e^{ky} \sin kx, \quad (2.76)$$

$$\sigma_{xy} = -\frac{\partial^2 U}{\partial x \partial y} = -Ak(1 + ky)e^{ky} \cos kx. \quad (2.77)$$

Performing the rotation of the coordinate system by the angle $\theta = \arctan y'(x)$ gives up to first order in Δ at the interface $y(x) = \Delta \sin kx$,

$$\sigma_{nn} = 0, \quad (2.78)$$

$$\sigma_{n\tau} = -(\Delta \sigma_0 + A)k \cos kx, \quad (2.79)$$

$$\sigma_{\tau\tau} = \sigma_0 + Ak(2 + ky)e^{ky} \sin kx. \quad (2.80)$$

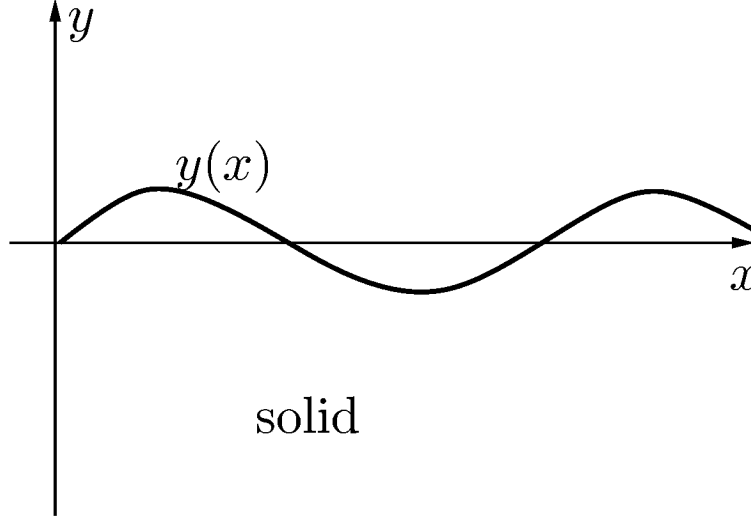


Figure 2.7: A solid with a sinusoidal surface profile. The original flat surface is located at $y(x) \equiv 0$.

Vanishing normal and shear stresses (we ignore surface tension) impose therefore the condition

$$A = -\Delta\sigma_0. \quad (2.81)$$

Consequently, the tangential stresses at the interface are

$$\sigma_{\tau\tau} = \sigma_0 - 2\Delta\sigma_0 k \sin kx. \quad (2.82)$$

The chemical potential is thus

$$\mu = \Omega\Delta \left(-2\frac{1-\nu^2}{E}\sigma_0^2 k + \alpha k^2 \right) \sin kx. \quad (2.83)$$

We introduce now a dynamic evolution for the surface profile. We assume that this surface diffusion process is slow and the application of the static theory of elasticity legitimate. Formally, the prefactor Δ becomes now time-dependent. The equation of motion is

$$\dot{y} = \frac{D}{\alpha\Omega} \mu'', \quad (2.84)$$

where the dot denotes $\partial/\partial t$ and the prime $\partial/\partial x$. D is the surface diffusion constant. The evolution of the amplitude is

$$\Delta(t) = \Delta_0 e^{\lambda t} \quad (2.85)$$

with

$$\lambda = Dk^2 \left(2\frac{1-\nu^2}{E\alpha}\sigma_0^2 k - k^2 \right). \quad (2.86)$$

We introduce the Grinfeld length

$$L_G := \frac{E\alpha}{2(1-\nu^2)\sigma_0^2}, \quad (2.87)$$

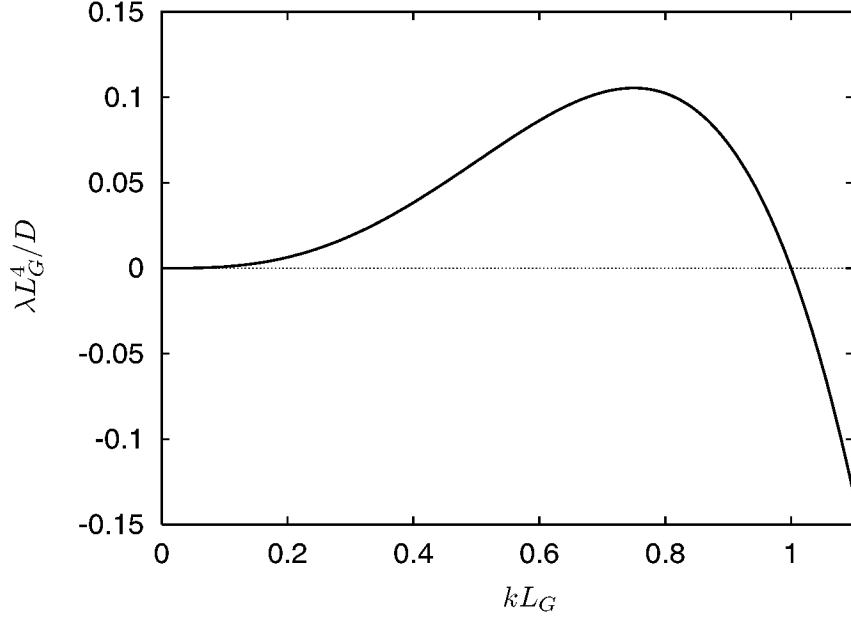


Figure 2.8: Spectrum of the Grinfeld instability. Long-wave perturbations are unstable.

and the spectrum is plotted in Fig. 2.8. The surface is stable against short-wave perturbations which are hampered by the surface energy, whereas it is unstable against long-wave distortions.

Under which circumstances is this analysis correct? The simplification of our calculations lies in the fact that we ignore time-dependencies in the solution of the elastic problem. The (nontrivial) part of the stress field is $\sigma \sim \Delta\sigma_0 k$, therefore $u_{ij} \sim \Delta\sigma_0 k/E$ and $u_i \sim u_{ij}/k \sim \Delta\sigma_0/E$. The inertial term is $\rho\ddot{u}_i \sim \rho\lambda^2\Delta\sigma_0/E$. For small values of k , the elastic contribution dominates the spectrum, thus

$$\rho\ddot{u}_i \sim \rho D^2 k^6 \Delta\sigma_0^5 E^{-3} \alpha^{-2}. \quad (2.88)$$

For $k \gg k_{Gr} \sim \sigma_0^2/E\alpha$,

$$\rho\ddot{u}_i \sim \rho D^2 k^8 \Delta\sigma_0/E. \quad (2.89)$$

We demand that $\rho\ddot{u}_i \ll \partial\sigma_{ij}/\partial x_j \sim \Delta\sigma_0 k^2$. This is always valid for sufficiently small diffusion coefficients. However, modes with big k decay so fast that dynamical effects become relevant and slow down the exponential decay.

Additionally, the boundary conditions change in a dynamical description and become (see section 7.1.1)

$$\begin{aligned} \sigma_{ni} &\sim v_n \rho \dot{u}_i \sim \Delta\lambda \rho u_i \lambda \\ &\sim \Delta^2 \lambda^2 \rho \sigma_0 / E. \end{aligned} \quad (2.90)$$

This effect is of quadratic order in Δ and can therefore be neglected. The same is true for the kinetic contribution to the chemical potential $\mu_{kin} \sim \Omega \rho \dot{u}_i^2$; furthermore, the potential contribution is indeed $\mu_{stat} \sim \Omega \sigma_{\tau\tau}^2 / E$.

2.8.4 The cusp singularity

So far we studied only the linear stability of a planar interface subjected to nonhydrostatic stress. Perturbations with a wavelength bigger than a critical value lead to a reduction of the total energy, and thus the configuration is unstable. If this instability develops in time, deep grooves can form (see Fig. 2.9) [40, 41, 19]; the lower elastic energy can also be read as easier deformability of the solid against the uniaxial loading.

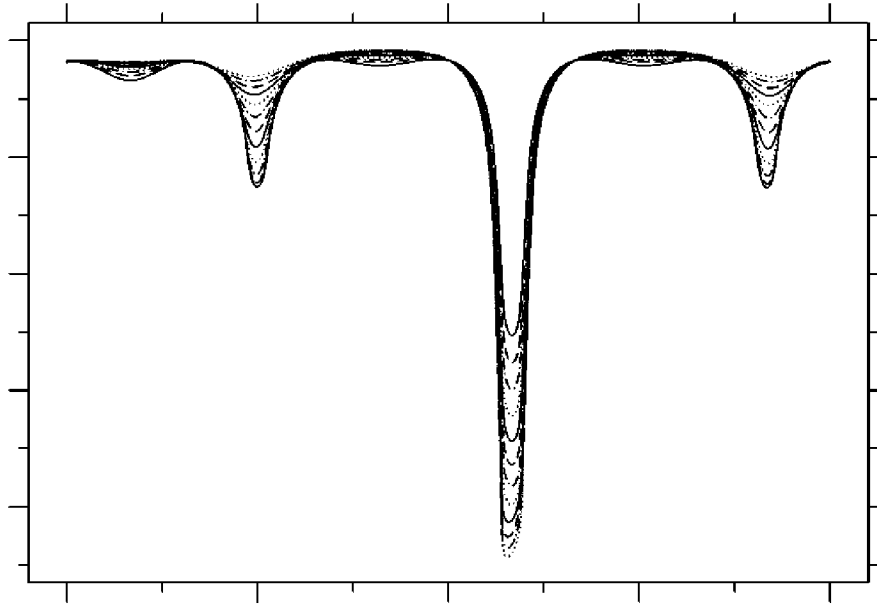


Figure 2.9: Formation of deep grooves caused by the Grinfeld instability. The picture shows a consecutive set of interface profiles; the tip radius in the notches decreases to zero and the propagation velocity finally diverges after a finite time. Notice that the physical process in this picture is not surface diffusion but melting and recrystallization of a solid below the interface line which is in contact with its melt phase [41].

It turns out that the propagation velocity of these notches increases in time and reaches infinity after a finite time. Simultaneously, the radius of curvature in the tip region of the grooves decreases to zero. Here, the physical description breaks down. In chapter 6 we work out the origin of the failure and develop a mechanism to overcome it; then the already mentioned link between the Grinfeld instability and the theory of fracture becomes much deeper.

2.9 Bending of thin plates

We consider a thin plate which is bent by the influence of different types of external forces. Obviously, some parts of the plate are compressed and others are stretched. Stretching happens on the convex side of the plate, and the magnitude of this elongation decreases towards deeper layers of the plate. Finally, the concave side is compressed; in between, there is a *neutral fiber*, which is located in the middle of the plate.

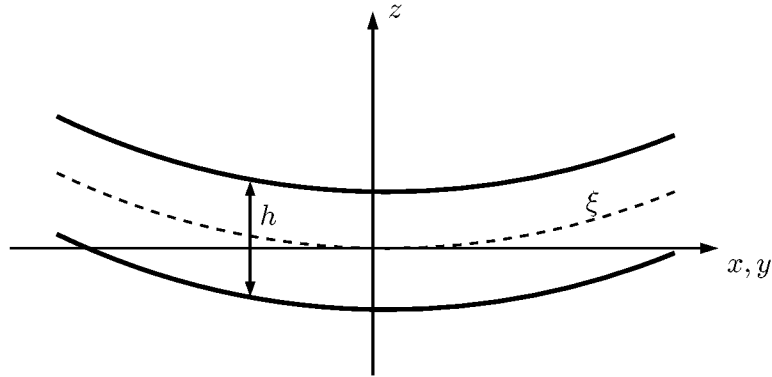


Figure 2.10: Cross section through a thin plate. The dashed line indicates the neutral fiber.

The undeformed plate is located in the xy plane, the neutral fiber being at $z = 0$. The vertical displacement of this fiber is denoted by ξ (see Fig. 2.10). Displacements within the

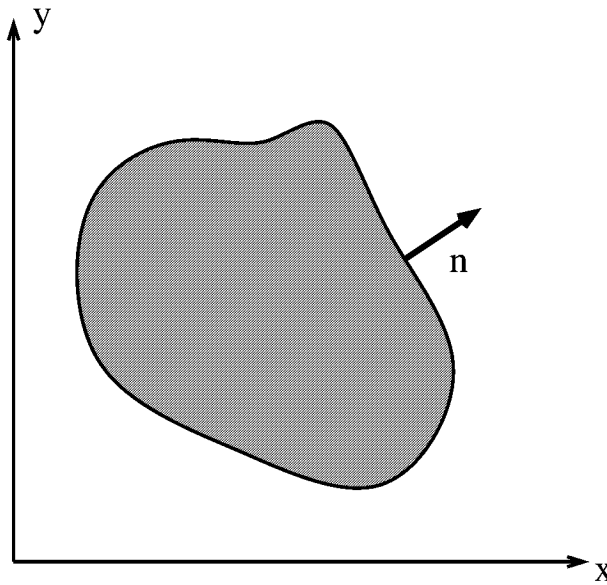


Figure 2.11: Definition of the normal vector for a thin plate in the x, y plane.

xy plane are small and of second order in the external force and can therefore be neglected. Thus, the displacement vector of the neutral fiber (0) is given by

$$u_x^{(0)} = u_y^{(0)} = 0, \quad u_z^{(0)} = \xi(x, y). \quad (2.91)$$

Since the plate is very thin, only weak forces are necessary to deform it. It turns out that the internal stresses due to stretching and compression are much bigger. Consequently, from boundary conditions, we have approximately $\sigma_{xz} = \sigma_{yz} = \sigma_{zz} = 0$ in the whole plate.

The elastic free energy, which is stored in the bent plate, is calculated in [42],

$$F_{pl} = \frac{Eh^3}{24(1-\nu^2)} \iint \left\{ \left(\frac{\partial^2 \xi}{\partial x^2} + \frac{\partial^2 \xi}{\partial y^2} \right)^2 + 2(1-\nu) \left[\left(\frac{\partial^2 \xi}{\partial x \partial y} \right)^2 - \frac{\partial^2 \xi}{\partial x^2} \frac{\partial^2 \xi}{\partial y^2} \right] \right\} dx dy, \quad (2.92)$$

with the thickness of the plate h . The surface integral is performed over the surface of the plate.

With the pressure P exerted on one side of the plate, the variation condition for the displacement $\delta \xi$,

$$\delta F_{pl} - \iint P \delta \xi dx dy = 0 \quad (2.93)$$

has to be fulfilled. Variation of (2.92) leads to a bulk and a boundary contribution. The first one gives

$$\iint (D \Delta^2 \xi - P) \delta \xi dx dy = 0, \quad (2.94)$$

with independent variations $\delta \xi$ and the stiffness coefficient

$$D = \frac{Eh^3}{12(1-\nu^2)}. \quad (2.95)$$

Therefore, one obtains the fourth order differential equation

$$D \Delta^2 \xi = P \quad (2.96)$$

for the vertical displacements.

The variation of the boundary contribution to (2.92) gives the boundary condition for ξ . For the case of force free boundary elements, this leads to a complicated set of equations on the perimeter of the plate (see [42]). The case of fixed edges gives the easier and obvious conditions

$$\xi = 0, \quad \frac{\partial \xi}{\partial n} = 0, \quad (2.97)$$

where n denotes the normal of the plate boundary (see Fig. 2.11).

Chapter 3

Grinfeld instability with surface tension

In this chapter we study how elasticity is affected by *surface tension*. Emphasizing that *surface energy* and *surface tension* are different properties of a system, we derive the modified chemical potential and the corrected boundary conditions. For this, we perform a variation calculation from an energy functional in order to establish a consistent way to derive the fundamental equations. In a later chapter, we will use a similar approach to include dynamical effects. Finally, in sections 3.4 and 3.5, we calculate the spectrum of the Grinfeld instability, now including also surface tension. The same was already done by Grilhe [34], but he receives an incorrect result. Here we rectify this mistake.

3.1 Surface energy and surface tension

In our calculations we took so far only *surface energy* into account. This means that we used the functional

$$W = \frac{1}{2} \int_V \sigma_{ij} u_{ij} dV + \int_{\partial V} \alpha d\tau, \quad (3.1)$$

where V is the volume of integration, ∂V its boundary and $d\tau$ an infinitesimal tangential element of this boundary. We point out that the *surface energy* contribution expresses the energy of the *undeformed* surface, not including displacements. From this term all basic equations can be derived by variational procedures. Here we give only the results which were already obtained in the first chapter or are special cases of calculations later in this chapter.

From a variation with respect to displacements, we gain the elastic equations

$$\frac{\partial \sigma_{ij}}{\partial x_j} = 0, \quad (3.2)$$

$$\sigma_{in} = 0, \quad (3.3)$$

with the surface normal n (see Fig. 3.1). We remark that the second equation results from a variation of the displacement u_i at the boundary. Since there is no contribution from the second integral in (3.1) which contains u_i , the resulting equation is homogeneous.

The chemical potential at the surface is up to a factor Ω of the atomic volume given by the energy density

$$\mu = \Omega \left(\frac{1}{2} \sigma_{ik} u_{ik} - \alpha \kappa \right). \quad (3.4)$$

Surface tension reflects that the total area of the surface changes also due to elastic displacements. Elongation of the surface e.g. by external forces leads to an additional compressive force. But even without external loading a self-stress can be present, for example in a balloon filled with air.

The elongation of an interface element $d\tau$ is proportional to the tangential strain, $u_{\tau\tau}d\tau$. Therefore the energy functional reads now

$$W = \frac{1}{2} \int_V \sigma_{ij} u_{ij} dV + \int_{\partial V} \alpha d\tau + \int_{\partial V} \beta u_{\tau\tau} d\tau. \quad (3.5)$$

The coefficient β is called *surface tension*. Usually α and β are of the same order of magnitude; for a liquid they are even equal [50]. One important observation is that the last surface integral contains now also the elastic fields, and thus one can expect that an inhomogeneous contribution can appear in the elastic boundary conditions. This and also the modified chemical potential will be derived in the next sections.

In the *full* thermodynamical equilibrium, the surface of a solid body is stress free. Then surface energy and surface tension describe the same effect. However, in many situations not all degrees of freedom of a system have relaxed to the full equilibrium; in this state of a local equilibrium which can be stable for long times, a precise discrimination between surface energy and surface tension is necessary and detailed specifications of the model situation are unavoidable.

3.2 Derivation of the chemical potential

If additionally to elastic effects and surface *energy*, surface *tension* is introduced, the expression for the chemical potential changes as well. Assume that in xy representation the interface is given by a function $y(x)$ (see Fig. 3.1). The chemical potential is the energy density at the surface, or, in other words and more generally,

$$\mu(x) = \Omega \frac{\delta W}{\delta y(x)}. \quad (3.6)$$

This allows to derive the curvature contribution and also the more complicated surface tension contribution to the chemical potential.

We start very generally from the functional

$$W[y] = \int f(x, y(x), y'(x)) \sqrt{1 + y'^2(x)} dx. \quad (3.7)$$

Surface energy is given by

$$f_\alpha = \alpha, \quad (3.8)$$

and the surface tension energy by the tangential strain

$$f_\beta = \beta u_{\tau\tau}. \quad (3.9)$$

We obtain the functional derivative

$$\frac{\delta W}{\delta y} = - \left[f \frac{y'}{(1 + y'^2)^{1/2}} \right]' + \frac{\partial f}{\partial y} \sqrt{1 + y'^2} - \left[\frac{\partial f}{\partial y'} \sqrt{1 + y'^2} \right]'$$

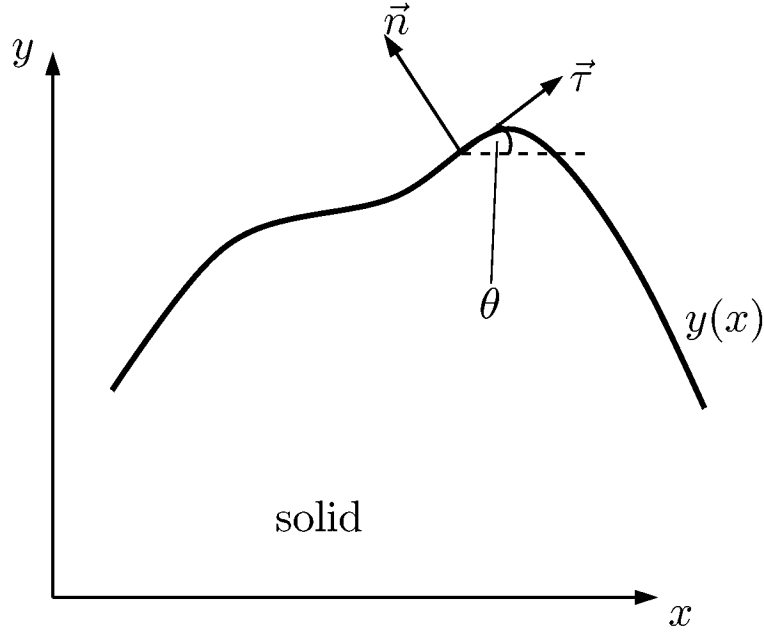


Figure 3.1: Derivation of the chemical potential. The solid phase is located below the interface line $y(x)$.

$$\begin{aligned}
 &= - \left(\frac{\partial f}{\partial x} + \frac{\partial f}{\partial y} y' + \frac{\partial f}{\partial y'} y'' \right) \frac{y'}{(1+y'^2)^{1/2}} - f \cdot \left(\frac{y''}{(1+y'^2)^{1/2}} - \frac{y'^2 y''}{(1+y'^2)^{3/2}} \right) \\
 &\quad + \frac{\partial f}{\partial y} (1+y'^2)^{1/2} - \left(\frac{\partial^2 f}{\partial y' \partial x} + \frac{\partial^2 f}{\partial y \partial y'} y' + \frac{\partial^2 f}{\partial y'^2} y'' \right) (1+y'^2)^{1/2} \\
 &\quad - \frac{\partial f}{\partial y'} \frac{y' y''}{(1+y'^2)^{1/2}}.
 \end{aligned}$$

Curvature is given by

$$\kappa = \frac{y''}{(1+y'^2)^{3/2}}, \quad (3.10)$$

and we have normal and tangential vectors

$$\vec{n} = \frac{1}{(1+y'^2)^{1/2}} \begin{pmatrix} -y' \\ 1 \end{pmatrix}, \quad \vec{\tau} = \frac{1}{(1+y'^2)^{1/2}} \begin{pmatrix} 1 \\ y' \end{pmatrix}. \quad (3.11)$$

Instead of Cartesian coordinates (x, y, y') (where y' is used to describe the slope), we use now local coordinates (n, τ, θ) . n is the normal, τ the tangential coordinate and θ the inclination angle of the interface. With

$$\theta = \arctan y', \quad (3.12)$$

we get the following transformation rules:

$$\left(\frac{\partial}{\partial \theta} \right)_{n, \tau} = (1+y'^2) \left(\frac{\partial}{\partial y'} \right)_{x, y}, \quad (3.13)$$

$$\left(\frac{\partial}{\partial n}\right)_{\tau,\theta} = \frac{-y'}{(1+y'^2)^{1/2}} \left(\frac{\partial}{\partial x}\right)_{y,y'} + \frac{1}{(1+y'^2)^{1/2}} \left(\frac{\partial}{\partial y}\right)_{x,y'}, \quad (3.14)$$

$$\left(\frac{\partial}{\partial \tau}\right)_{n,\theta} = \frac{1}{(1+y'^2)^{1/2}} \left(\frac{\partial}{\partial x}\right)_{y,y'} + \frac{y'}{(1+y'^2)^{1/2}} \left(\frac{\partial}{\partial y}\right)_{x,y'}. \quad (3.15)$$

Comparing this with the above expression gives the invariant formula

$$\frac{\delta W}{\delta y} = \left(\frac{\partial f}{\partial n}\right)_{\tau,\theta} - f \cdot \kappa - \left(\frac{\partial^2 f}{\partial \tau \partial \theta}\right)_n - \kappa \left(\frac{\partial^2 f}{\partial \theta^2}\right)_{n,\tau}. \quad (3.16)$$

The simplest case of surface energy leads immediately to the Gibbs-Thomson correction $\mu_s = -\Omega\alpha\kappa$.

For the surface tension correction, we have

$$f = u_{\tau\tau} = u_{ij}\tau_i\tau_j. \quad (3.17)$$

From (3.13) follows

$$\left(\frac{\partial f}{\partial \theta}\right)_{n,\tau} = 2u_{n\tau}, \quad \left(\frac{\partial^2 f}{\partial \theta^2}\right)_{n,\tau} = 2(u_{nn} - u_{\tau\tau}). \quad (3.18)$$

We also consider $u_{n\tau}(\tau) = u_{n\tau}(n=0, \tau, \theta(\tau))$ on the surface as function of the arclength parameter τ . Then we get for the total derivative

$$\begin{aligned} \frac{du_{n\tau}}{d\tau} &= \left(\frac{\partial u_{n\tau}}{\partial \tau}\right)_{n,\theta} \Big|_{n=0, \theta=\theta(\tau)} + \left(\frac{\partial u_{n\tau}}{\partial \theta}\right) \Big|_{n=0} \frac{d\theta}{d\tau} \\ &= \left(\frac{\partial u_{n\tau}}{\partial \tau}\right)_{n,\theta} \Big|_{n=0, \theta=\theta(\tau)} - \kappa(u_{\tau\tau} - u_{nn}). \end{aligned} \quad (3.19)$$

It contains both translational and rotational contributions. By boundary conditions, we have $u_{n\tau} = 0$ on the surface; however, only the *total* derivative (3.19) is zero, the translational contribution itself is not. Thus

$$\left(\frac{\partial^2 f}{\partial \theta \partial \tau}\right)_{n,\theta} \Big|_{n=0, \theta=\theta(\tau)} = -2\kappa(u_{nn} - u_{\tau\tau}). \quad (3.20)$$

Combining the preceding results, we obtain

$$\frac{\delta}{\delta y(x)} \int_{\partial V} u_{\tau\tau} d\tau = \left(\frac{\partial u_{\tau\tau}}{\partial n}\right)_{\tau,\theta} - u_{\tau\tau}\kappa. \quad (3.21)$$

This leads finally to the chemical potential

$$\mu_\beta = \Omega\beta \left[\left(\frac{\partial u_{\tau\tau}}{\partial n}\right)_{\tau,\theta} - u_{\tau\tau}\kappa \right]. \quad (3.22)$$

Summing up, if we start from the total energy

$$W = \int_V \frac{1}{2} \sigma_{ij} u_{ij} dV + \int_{\partial V} (\alpha + \beta u_{\tau\tau}) d\tau, \quad (3.23)$$

we obtain for the total chemical potential

$$\mu = \Omega \left(\frac{1}{2} \sigma_{ik} u_{ik} - \alpha\kappa + \beta \left[\left(\frac{\partial u_{\tau\tau}}{\partial n}\right)_{\tau,\theta} - u_{\tau\tau}\kappa \right] \right). \quad (3.24)$$

3.3 Derivation of the elastic equations and boundary conditions

The stationary elastic equations and the boundary conditions can be obtained by variation of the total energy (3.23) with respect to the displacement u_i (instead of variation with respect to the interface position in the previous section).

The tangential strain is given by

$$u_{\tau\tau} = \frac{du_\tau}{d\tau} - u_n\kappa. \quad (3.25)$$

Therefore we obtain for the variation of the total energy

$$\delta W = - \int_V \frac{\partial \sigma_{ik}}{\partial x_k} \delta u_i dV + \int_{\partial V} \left(\sigma_{ni} \delta u_i + \beta \frac{d\delta u_\tau}{d\tau} - \beta \kappa \delta u_n \right) d\tau. \quad (3.26)$$

The second term in the interface integral is zero since it can be integrated along the closed boundary. From the variation in the interior we get the static equations

$$\frac{\partial \sigma_{ik}}{\partial x_k} = 0, \quad (3.27)$$

from the variation at the rim the boundary conditions

$$\sigma_{n\tau} = 0, \quad \sigma_{nn} = \beta\kappa. \quad (3.28)$$

3.4 Grinfeld instability with surface tension

We can also perform a stability analysis of a slightly perturbed interface which is subjected to an nonhydrostatic loading as in section 2.8.3; now we also take into account the modified boundary conditions (3.28) and the chemical potential (3.24). For the interface (2.73) we use the Airy function

$$U = \frac{\sigma_0^2 y^2}{2} + (Ay + B)e^{ky} \sin kx. \quad (3.29)$$

From the boundary conditions, we obtain to first order in Δ

$$A = -\Delta(\beta k + \sigma_0), \quad B = \beta\Delta. \quad (3.30)$$

The total chemical potential (3.24) at the interface is therefore

$$\mu = \Omega \left(\frac{(1 - \nu^2)\sigma_0^2}{E} + k\Delta \sin kx \left[-2\sigma_0^2 \frac{1 - \nu^2}{E} + \alpha k - k \frac{\beta(1 - \nu^2)}{E} (3\sigma_0 + 2\beta k) \right] \right). \quad (3.31)$$

The resulting spectrum of surface diffusion is ($k \geq 0$)

$$\lambda = Dk^3 \left(2\sigma_0^2 \frac{1 - \nu^2}{E\alpha} - k + k \frac{\beta(1 - \nu^2)}{E\alpha} (3\sigma_0 + 2\beta k) \right). \quad (3.32)$$

Obviously, the surface tension favors the Grinfeld instability. Apart from the Grinfeld length

$$L_G = \frac{E\alpha}{2(1 - \nu^2)\sigma_0^2}, \quad (3.33)$$

we have now an additional lengthscale in the system

$$L_\beta := \frac{\beta}{\sigma_0}. \quad (3.34)$$

Consequently, the spectrum can be expressed as

$$\lambda L_G^4/D = (kL_G)^3 \left(1 - (kL_G) + \frac{3}{2}(kL_G) \frac{L_\beta}{L_G} + (kL_G)^2 \frac{L_\beta^2}{L_G^2} \right). \quad (3.35)$$

Typically, $L_\beta \ll L_G$, since $\sigma_0 \ll E$, and thus the surface tension correction can be neglected. However, the self-stress due to surface tension in Eq. (3.32) leads to an instability even without external loading σ_0 .

3.5 The energetic approach

We also compare the energy of the solid with flat surface to the energy of the corrugated solid. This confirms independently the results from the previous section.

We calculate the energy according to Eq. (3.23), which is contained in a strip of width $2\pi/k$ (one period). Notice that the amount of material in this strip is exactly the same as in the solid with flat surface.

The elastic energy density is

$$w_{el} = \frac{1}{2} \sigma_{ij} u_{ij}. \quad (3.36)$$

The total elastic energy,

$$W_{el} = \int_{x=0}^{2\pi/k} \int_{y=-\infty}^{y(x)} w_{el} dy dx, \quad (3.37)$$

is infinite due to the zeroth order contribution, and therefore we immediately subtract it. The second order contribution in Δ is

$$W_{el}^{(2)} = -\frac{\pi \Delta^2}{E} (1 - \nu^2) (\sigma_0^2 - k^2 \beta^2). \quad (3.38)$$

The surface energy is

$$W_s = \int_{x=0}^{2\pi/k} \alpha \sqrt{1 + y'^2} dx, \quad (3.39)$$

which is to second order

$$W_s^{(2)} = \frac{\alpha k \pi \Delta^2}{2}. \quad (3.40)$$

Finally, the surface tension contribution

$$W_\beta = \int_{x=0}^{2\pi/k} \beta u_{\tau\tau} \sqrt{1 + y'^2} dx \quad (3.41)$$

gives

$$W_\beta^{(2)} = -\frac{\beta k \pi \Delta^2}{2E} (1 - \nu^2) (4k\beta + 3\sigma_0). \quad (3.42)$$

Altogether, $W^{(2)} = W_{el}^{(2)} + W_s^{(2)} + W_\beta^{(2)}$ results in

$$W^{(2)} = \frac{\pi\Delta^2}{2} \left(-2\sigma_0^2 \frac{1-\nu^2}{E} + \alpha k - k \frac{\beta(1-\nu^2)}{E} (3\sigma_0 + 2k\beta) \right). \quad (3.43)$$

This results confirms the spectrum (3.32) and corrects the expression in [34]. Notice that the the Poisson ratio appears only in the combination $1 - \nu^2$; this is the only allowed form in plane strain configurations.

3.6 Summary

In this chapter we analyzed the influence of surface tension on the Grinfeld instability. We started with a derivation of all necessary equations from the functional

$$W = \int_V \frac{1}{2} \sigma_{ij} u_{ij} dV + \int_{\partial V} \alpha d\tau + \int_{\partial V} \beta u_{\tau\tau} d\tau. \quad (3.44)$$

From this we obtain modified elastic boundary conditions, $\sigma_{nn} = \beta\kappa$, which can lead to a self-stress. The chemical potential is also modified, and consequently the spectrum of the Grinfeld instability, too. In most cases, the influence of the surface tension can be neglected in the initial stage of the instability. However, it leads to a de-stabilization even without external nonhydrostatic loading.

Chapter 4

Coarsening kinetics with elastic effects

4.1 Introduction

The growth of crystals from the melt or from a solution are typical examples of first-order phase transitions. Ostwald ripening is the late-stage process by which a new phase coarsens in order to lower the interfacial free energy. During this process the characteristic length scale of the precipitates increases in time, the supersaturation decreases and the system moves towards phase equilibrium.

The classical coarsening theory was given by Lifshitz, Slyozov and Wagner (LSW) [47, 78] in the framework of a mean-field approach which is valid in the limit of small volume fractions of the new phase. In this approach all precipitated particles are assumed to be spherical and remote from each other. If the diffusional transport of mass or heat is the limiting kinetics of the process, the average size of the particles grows with a power law in time with an exponent of $1/3$. The particle distribution function shows a characteristic scaling behavior.

In this chapter we demonstrate that long-range elastic effects lead to a complete change of this mean-field theory and cause different coarsening laws.

Strong elastic and thermal interactions between neighboring precipitates and the appearance of several relevant lengthscales destroy the “classical” behavior. Though the general evolution of the system becomes more complicated, it is quite surprising that under certain geometrical conditions still analytical predications are possible. As an example, we study here the melting of an superheated solid phase in which liquid inclusions appear. These inclusions are generically flat and not spherical; for a strong anisotropy they align along the crystallographic axes and coarsen in time.

In section 4.2 we give a short introduction to the conventional LSW theory. In section 4.3 we argue that elastic effects alter the behavior so strongly that this mean field theory cannot hold consistently.

In the sections 4.4 and 4.5 a new type of scaling laws is derived for the coarsening process with elastic effects in a layer structure.

This chapter is published in [10].

4.2 Ostwald ripening and the LSW theory

Here we give a very simplified derivation of the scaling laws of the standard Ostwald ripening process [51]. We refrain from deriving the explicit form of the particle size distribution function here [43].

Let us study in particular the dynamic evolution of an overheated solid with temperature T slightly higher than the melting temperature. During the initial nucleation phase, small melt precipitates appear by fluctuations. In the next stage, the growth phase, these nuclei grow; they use the (dimensionless) overheating $\Delta = c_p(T - T_M)/L_p$ (c_p is the heat capacity and L_p the latent heat) of the environment to melt the solid phase. Thus the precipitates grow and the average temperature approaches T_M . In this chapter, we concentrate on the following third stage, the coarsening regime. Whereas so far all nuclei were almost independent, they compete now for the remaining overheating. As an effect, larger particles grow at the expense of smaller ones which shrink and finally disappear. The mean size of the precipitates grows, their number decreases, until finally only one melt inclusion remains (see Fig. 4.1).

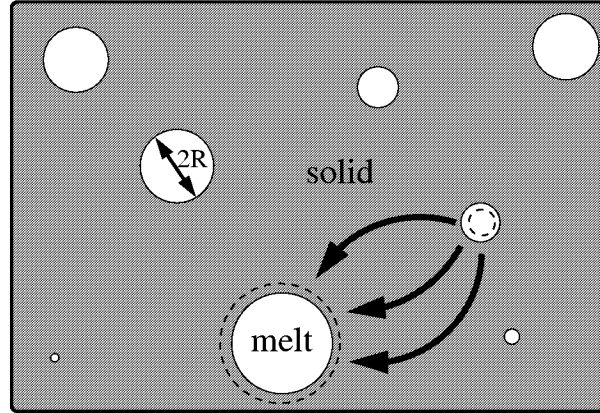


Figure 4.1: During the coarsening of the overheated solid, bigger precipitates grow at the expense of smaller ones by a diffusive heat transport through the matrix. The average particle size R increases in time and the number decreases.

Since the initial overheating is assumed to be small, the volume fraction of the new phase is also small. All dynamics result from diffusive heat transport between the inclusions.

The main assumption of the LSW theory is that only one lengthscale, the mean size R of the inclusions, is relevant in the system. It does not take into account long-range interactions like elastic forces and is valid only for relatively low overheatings.

At the interface of one (spherical) precipitate, the local overheating is given by the Gibbs-Thomson correction of surface energy, assuming local equilibrium,

$$\Delta_{int} = \frac{(T_{int} - T_M)c_p}{L_p} \sim \frac{d_0}{R}, \quad (4.1)$$

with the capillary length

$$d_0 \sim \frac{\alpha T_M c_p}{L_p^2}. \quad (4.2)$$

Here α is the surface energy density. The gradient of temperature compared to its average surrounding value drives a volume heat flux

$$j \sim D \frac{\Delta_{int}}{R}, \quad (4.3)$$

with the diffusion coefficient D . Heat conservation requires

$$\frac{d}{dt} (R^3) \sim j R^2, \quad (4.4)$$

which finally leads to the growth law

$$R \sim (d_0 D t)^{1/3}. \quad (4.5)$$

This is the famous scaling law of the Ostwald ripening, found by Lifshitz, Slyozov and Wagner. It is also valid for many other processes, e.g. the growth of precipitates from a supersaturated solution.

4.3 Breakdown of the classical theory

Novel aspects of kinetics of phase transitions appear if the initial metastable phase is a crystal. Generally, it is known that long-range elastic fields, which are inevitable in this situation, destroy the universal features of LSW growth, allowing other kinetics (see for example [60] and references therein). An oblate shape of the inclusions is often observed in experiments [64, 55, 29] and in computer simulations [60, 80, 79].

Due to a difference in the densities of the two cooperating phases, part of the crystal surrounding a particle of the new phase becomes deformed if the slow diffusion of the point defects is neglected. This modifies the system's behavior in comparison to an unstressed situation. If one assumes incoherence at the interface, as is definitely the case for the melting process or for gas inclusions, the precipitates have an oblate shape which is more favorable compared to a spherical shape because of its lower elastic energy. It immediately introduces an additional lengthscale to the problem, the height $h \ll R$ of the particles. This effect leads to a substantial modification of the laws of nucleation and growth [7, 9].

The main purpose of this chapter is to describe the last coarsening stage of this process which should also be very different from the one of classical LSW theory. The system inevitably arrives at a stage where the characteristic size of the particles is comparable to the distance between them. Indeed, if one assumes that these particles are very oblate lentils of radius R , height $h \ll R$ and distance L between them, the volume fraction $\Delta_0 \sim h R^2 / L^3$ should remain almost constant during the coarsening stage. On the other hand, if particles are well separated ($L \gg R$), according to Ref.[7], $h \sim R \Delta$ where Δ is the dimensionless supersaturation parameter which decreases with time. Then the ratio $R/L \sim (\Delta_0 / \Delta)^{1/3}$ becomes large in contradiction to the initial assumption $L \gg R$. This situation is very different from the case of spherical particles where, if the volume fraction Δ_0 is small, the ratio $R/L \sim \Delta_0^{1/3}$ remains small during the entire coarsening stage. Thus, for an oblate shape of inclusions the usual mean-field approximation has to be modified in order to account for several independent length scales and strong diffusional and elastic interactions between particles have to be taken into account. In the general case this problem is very difficult and we restrict our consideration to uniaxial crystals where the anisotropy orients the particles parallelly (see Fig. 4.2).

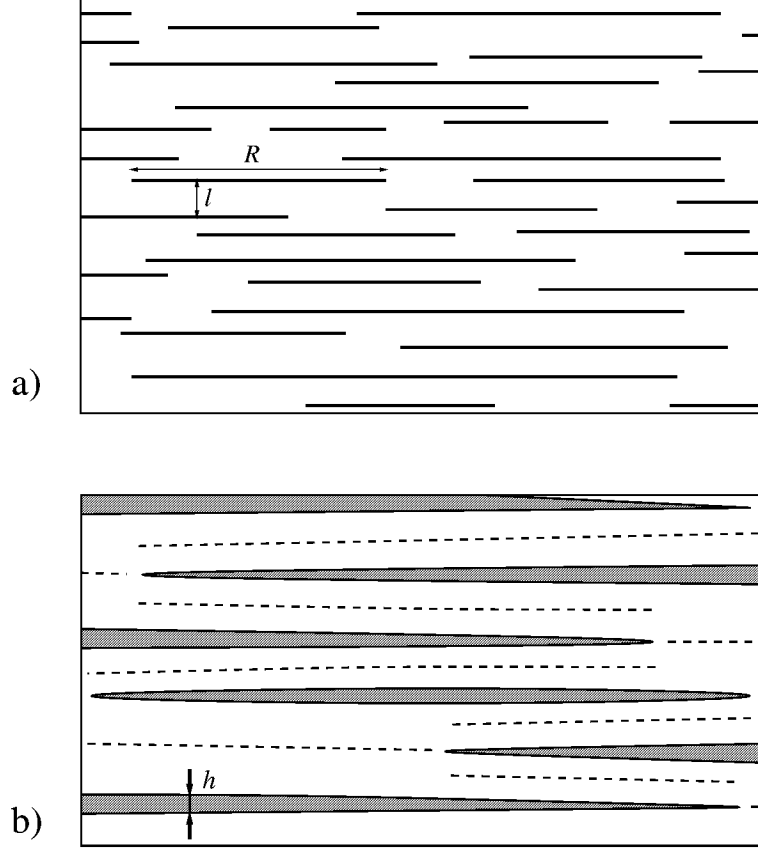


Figure 4.2: Cross section of the arrangement of liquid inclusions in the solid phase. b) is a magnified detail of a); the dashed lines indicate the center lines of the bent plates.

4.4 Coarsening in a layer structure

We assume that the new phase is a homogeneous melt with a chemical potential μ and pressure P (the external pressure is zero). The melting process of crystals is usually initiated at heterogeneous sites such as grain boundaries or free surfaces [16]. However, crystals can be superheated above the equilibrium melting point, provided heterogeneous nucleation is avoided by means of experimental techniques [21, 82]. Motion of a growing interface in this case is governed by the interplay between the irreversible diffusion of the latent heat (diffusional growth) and the reversible work done during elastic deformation and the formation of a new surface area.

The inclusions of the new phase are assumed to be very oblate lentils of characteristic lateral extent R and mean height $h \ll R$. Due to the density difference elastic deformations are necessarily present in the solid phase. The mass conservation law reads

$$(v_L - v_s)R^2h/v_s \sim W_d = \int u_n ds, \quad (4.6)$$

where v_L and v_s are the atomic volumes of the liquid and solid phases, and W_d is the deformation volume (u_n is the normal component of the displacement vector at the interface).

Solving the elastic problem, we can, in first approximation, ignore the height of the lentil. In this case the pressure P , exerted on the crystal by the liquid, is given on a plane cut within the mean radius R . If the particles of the new phase are well separated, this problem is equivalent to the crack problem and the normal component of the displacement vector at the interface is given by solution of that problem (see for example [69, 59]). The analogy to the crack problem has been used in previous publications [7, 9] concerning the analysis of the thermodynamics and growth of an isolated particle. However, in the present case the distance between particles is smaller than their size R and the elastic problem should be significantly modified compared to the usual crack problem.

4.5 The scaling behavior

We restrict our considerations to some simple order-of-magnitude estimates for the case of lentil shaped inclusions which are piled up to a layer structure as sketched in Fig. 4.2a.

Apart from radius and height of each lentil a new length scale, the distance between inclusions l in vertical z direction, is introduced. Our goal is to calculate the coarsening with time of all three mentioned length scales during the last stage of phase separation. The strategy is as follows: By solving the elastic problem and using the mass conservation law and the local equilibrium condition at the interface, we estimate the pressure P and the characteristic temperature at the interface as functions of the introduced length scales. Then estimating the existing gradients of temperature, we eventually find the growth law of a characteristic particle.

We confine our considerations to the case $R \gg l \gg h$ and will check the self-consistency of this assumption later. The pressure P_i inside the i -th particle depends on its size and on the geometry of the neighborhood. Let us denote the average pressure over the system of particles as $\langle P \rangle$. To estimate the stresses in the crystal in the considered layered structure, using the linearity of the theory of elasticity, we write the displacement field as a sum of three fields: $\mathbf{u} = \mathbf{u}^{(1)} + \mathbf{u}^{(2)} + \mathbf{u}^{(3)}$. The first field $\mathbf{u}^{(1)}$ corresponds to the uniaxial stress of the crystal, $\sigma_{zz} = -\langle P \rangle$. The other components of the stress field are zero. The second field $\mathbf{u}^{(2)}$ satisfies the condition of zero normal and shear stresses at the solid-liquid interfaces and compensates the stresses due to the $\mathbf{u}^{(1)}$ field in order to fulfill the condition of vanishing external pressure. The field $\mathbf{u}^{(2)}$ corresponds to the field of a network of springs schematically depicted by the dashed lines in Fig. 4.2b. Finally, the field $\mathbf{u}^{(3)}$ satisfies the boundary conditions $\sigma_{zz}^{(i)} = -(P_i - \langle P \rangle)$ at the interfaces of the particles.

To estimate the displacement fields $\mathbf{u}^{(2)}$ and $\mathbf{u}^{(3)}$ we can use the theory of elasticity of thin plates, since the ratio l/R is small (see section 2.9). For the field $\mathbf{u}^{(2)}$ the problem reduces to one for the u_z component of the centerline displacement (dashed lines in Fig. 4.2b) for each plate:

$$\frac{El^3}{12(1-\nu^2)}\Delta^2 u_z(x, y) = 0. \quad (4.7)$$

Here $\Delta = \partial_x^2 + \partial_y^2$ is the two-dimensional Laplacian; ν and E are the Poisson and Young coefficients. The problem for the field $\mathbf{u}^{(3)}$ reduces to the local problem of a plate bent due to the pressure difference $\delta P = P_i - P_j$ at opposite sides of the plate:

$$\frac{El^3}{12(1-\nu^2)}\Delta^2 u_z(x, y) = \delta P. \quad (4.8)$$

Eqs. (4.7) and (4.8) are subject to the natural boundary conditions at the lines connecting three plates of different thickness (at the edges of the inclusions): continuous displacements and orientations of all three plates and vanishing total force and torque acting on the triple junction from all three plates [42]. If we assume that the characteristic pressure difference δP is of the same order as the average pressure, then both fields are of the same order

$$u_z \sim P \frac{1 - \nu^2}{El^3} R^4 \quad (4.9)$$

and the corresponding deformation volume is

$$W_d \sim P \frac{1 - \nu^2}{El^3} R^6. \quad (4.10)$$

Basically Eq. (4.9), (4.10) can be understood as a scaling analysis of the elastic situation. Indeed, in the framework of linear theory of elasticity the displacement must be linear in P and, since Young's modulus appears only in the combination El^3 in bending problems, u_z must have the structure (4.9) in order to have the right units.

We assume local equilibrium conditions at the interface which relate the interface temperature and the pressure P inside the particle (Clausius-Clapeyron relation):

$$\Delta_{int} = \frac{(T_{int} - T_M)c_p}{L_p} = \frac{P(v_L - v_s)T_M c_p}{L_p^2 v_s}, \quad (4.11)$$

where we have neglected elastic and capillary corrections [7, 9]; Δ_{int} is the dimensionless interface superheating; T_M is the melting temperature at zero pressure P ; c_p and L_p are the specific and latent heat, respectively.

The edge of the crack-like inclusion is singular. The condition of local equilibrium also requires an additional variation of the free energy

$$\Delta F = -\frac{1}{2}PW_d + \alpha S \quad (4.12)$$

with respect to R [7, 9], where α is the surface energy and $S \sim R^2$ the area of the inclusion. This results in

$$P \frac{dW_d}{dR} \sim R\alpha. \quad (4.13)$$

The last expression is just a generalization of the Griffith condition for cracks to our case. It is a very important ingredient of our theory which allows us to relate the pressure P to the characteristic length scales of the problem. Now, using this condition (4.13) together with the solution of the elastic problem, Eq. (4.10), and with the mass conservation law, Eq. (4.6), we can find a relation between the different length scales of the problem:

$$h \sim \frac{\rho^{1/2} R^2}{l^{3/2}}, \quad (4.14)$$

where the microscopic length scale

$$\rho = \alpha(1 - \nu^2)v_s^2/[E(v_L - v_s)^2]$$

depends only on material parameters. On the other hand, using the local equilibrium condition, Eq. (4.11), we can present the interfacial superheating in the following form:

$$\Delta_{int} \sim \frac{d_0}{h} \frac{W_d}{W'_d R}, \quad (4.15)$$

where $d_0 = \alpha T_M c_p / L_p^2$ is the capillary length. This is quite a remarkable result: Since the ratio $W_d / (W'_d R)$ is just a number, the interface superheating is basically of capillary origin and depends only on the height h of the inclusion. In other words, the result formally looks like the Gibbs-Thomson correction for the curved interface with curvature of the order $1/h$. However the real curvature at the smooth part of the interface is of order h/R^2 and has been neglected. Therefore, the result is basically due to the Griffith condition and not a consequence of the Gibbs-Thomson correction in its usual meaning.

Furthermore the number of inclusions per unit volume behaves like $n \sim R^{-2} l^{-1}$ and thus, by global heat conservation, $n R^2 h \sim \Delta_0$, which results in the simple expression

$$h/l \sim \Delta_0, \quad (4.16)$$

where Δ_0 is the initial superheating of the crystal.

The growth kinetics is controlled by thermodiffusion. The temperature field in the solid phase obeys the diffusion equation and the following boundary conditions:

$$D \nabla^2 w = \partial w / \partial t, \quad (4.17)$$

$$v_n = D \vec{n} \cdot \nabla w|_{int}, \quad (4.18)$$

$$w|_{int} = \Delta_{int} \sim d_0/h. \quad (4.19)$$

Here $w = (T - T_M) c_p / L_p$ is the rescaled temperature field, measured from the melting temperature T_M ; D is the thermal diffusion constant. A melting front absorbs latent heat that diffuses as expressed by (4.17); the requirement of heat conservation at the interface gives (4.18) ($\vec{n}$ is the normal to the interface and v_n is the normal velocity). Eq. (4.19) is the local equilibrium condition (4.15). Under this condition, the field w inside the melt is constant and equal to its interfacial value (4.15). The bigger particles are less overheated and grow to the expense of the smaller ones. It is clear from Fig. 4.2 that the characteristic gradients of temperature are of the order Δ_{int}/l , and the continuity equation (4.18) together with the relation (4.16) gives the evolution law for the characteristic height h of the particle:

$$\dot{h} \sim D d_0 \Delta_0 / h^2. \quad (4.20)$$

This evolution equation is qualitatively close to the corresponding one in the classical LSW theory and leads to the coarsening law

$$h(t) \sim (\Delta_0 d_0 D t)^{1/3} \quad (4.21)$$

with the same scaling exponent $1/3$. However, there is an important difference between these two cases. First of all, our evolution equation is nothing but an order-of-magnitude estimate. In fact we deal with a many particle problem where the local gradients depend on the structure of the close neighborhood and not on the mean-field temperature. On the other hand, the mean-field approach for spherical particles is exact for small volume fractions Δ_0 . Secondly,

this small volume fraction enters into the final scaling, Eq. (4.21), which makes the coarsening process in our case slower than for the spherical particles.

Using Eq. (4.15), we find that the superheating of the system decreases as:

$$\Delta(t) \sim d_0^{2/3} / (\Delta_0 D t)^{1/3}. \quad (4.22)$$

Of course, the coarsening stage corresponds to the time range when $\Delta(t) \ll \Delta_0$. Finally, the coarsening laws for the other length scales of the problem, l and R , can be found from Eq. (4.16) and (4.14), respectively:

$$l(t) \sim (d_0 D t)^{1/3} \Delta_0^{-2/3}, \quad (4.23)$$

$$R(t) \sim l(t) (d_0 / \rho)^{1/4} [\Delta_0 / \Delta(t)]^{1/4} \sim t^{5/12}. \quad (4.24)$$

We note that the elastic properties and the density difference enter only into the scaling for the radius R through the microscopic length scale ρ . Eqs. (4.21)-(4.24) are the main results of this chapter.

Let us discuss the consistency of the used approximations. First of all, the basic assumption about the hierarchy of the length scales involved, $R \gg l \gg h$, is clearly valid for small initial superheating $\Delta_0 \ll 1$. Secondly, we have used the hydrostatic approximation and have neglected the viscous flow necessarily present inside the inclusions due to mass redistribution. The characteristic difference in pressure, arising from the viscous flow with the velocity of the order of $\dot{R}$, is $\delta P \sim \eta \dot{R} R / h^2$ where η is the viscosity. In the coarsening stage this pressure is small compared to the hydrostatic pressure,

$$\frac{\delta P}{P} \sim \frac{\eta D (v_l - v_s)}{\alpha v_s} \frac{1}{h(t)} \left(\frac{d_0}{\rho} \right)^{1/2} \left(\frac{\Delta(t)}{\Delta_0} \right)^{1/2} \ll 1,$$

since $h(t)$ grows and $\Delta(t)$ decays in time. Thus, the used hydrostatic approximation is legitimate.

The smooth shape of a growing nucleus should undergo a Mullins-Sekerka instability. In the usual case of the spherical nucleus this happens when the radius of the nucleus becomes a few times larger than the critical radius [53]. However, this instability is irrelevant in the coarsening regime since all important radii in the distribution function are still stable. In our case of oblate inclusions the Mullins-Sekerka length is $\lambda_{MS} \sim (d_0 D / \dot{h})^{1/2} \sim (l h)^{1/2}$ and one may naively expect the development of an instability. However, the perturbation grows in time as $\exp(\gamma t)$, where γ itself decays in time as $\gamma \sim \dot{h} / \lambda_{MS} \sim \Delta_0^{1/2} / t$. Thus, $\gamma t \sim \Delta_0^{1/2}$ never becomes large and the instability is not important.

Our results should be relevant to other types of phase transitions inside a solid phase. The coarsening of gaseous crack-like pores (see, for example, [77] and references therein) requires diffusion of the impurities towards the crack, while elastic deformations arise due to the non-vanishing gas volume and pressure. We also mention the transition of a metastable metallic crystal phase into an insulating amorphous state. This process, analyzed in [29] by a stepwise annealing to investigate the temperature dependence of the conductivity of the emerging two-phase material, is also accompanied by an increase of specific volume. Based on resistance measurements the authors draw the conclusion that the growing amorphous phase has a very oblate shape.

4.6 Summary

In this chapter we studied the coarsening of melt inclusions in a overheated solid matrix. In this latest regime of the first order phase transition to its equilibrium configuration, the average size of the inclusions increases and their number decreases. Bigger precipitates grow at the expense of smaller ones which shrink and finally disappear.

Elastic effects lead to strong diffusional and elastic interactions between neighboring inclusions and destroy the mean field behavior of the standard LSW theory. The particles are no longer spherical but have an oblate shape. Altogether, three different length scales become relevant in the system of a crystal with anisotropy, where all nuclei align in the same direction: the average size R of the inclusions (i.e. their lateral extend), their height h and their vertical distance h . These lengthscales obey the hierarchy $R \gg l \gg h$ and have coarsening laws

$$R \sim t^{5/12}, \quad l \sim h \sim t^{1/3}. \quad (4.25)$$

The dimensionless overheating decreases simultaneously as

$$\Delta \sim t^{-1/3}. \quad (4.26)$$

This leads finally in a consistent way to the thermodynamical equilibrium.

It is quite remarkable that in this system with strong thermal and elastic interactions and several lengthscales still analytical predictions are possible. One of the main ideas used here is the application of the theory of bending of thin plates. However, the situation is expected to become more complicated in systems without anisotropy; then complicated networks of crack-like melt inclusions can form. It is a very important challenge to understand these processes in the future.

Chapter 5

Coarsening of cracks in a uniaxially strained solid

5.1 Introduction

In the early theory of fracture, Griffith [33] developed a criterion which predicts the irreversible growth of a crack, provided a critical length is exceeded, and conversely its disappearance if it is shorter. The critical length depends on the external tension P in the sense that a higher tension leads to a lower threshold of instability. The origin of this instability is founded on a competition between a release of elastic energy, caused by the opening of the crack, and an increase of surface energy. The critical Griffith crack is analogous to the critical nucleus in a first order phase transition.

Statistical mechanics of cracks in the nucleation stage has been discussed in [14, 15] using this analogy between the theory of fracture and first order phase transitions. A solid is unstable against an external tension $P < 0$ because the true ground state of the system is fractured into pieces. In a sense, a solid under stretching is similar to a supercooled gas: the point of zero external stress plays the role of the liquid-gas condensation point. During this nucleation stage all cracks are well separated and hence a dilute gas approximation of straight cracks in an infinite medium is legitimate.

However, the late stage of phase separation is characterized by Ostwald ripening when a new phase coarsens in order to lower the interfacial free energy. Larger droplets are energetically more favorable because of their smaller interface curvature. Thus they grow at the expense of smaller inclusions which resolve again and finally disappear. This collective behavior leads to a growth of the average droplet size and simultaneously to a decrease of their number (see section 4.2). Finally the system reaches the full thermodynamic equilibrium. The same coarsening process should take place in a system of cracks according to the analogy mentioned above. However, to our best knowledge, this problem has not been addressed in the literature so far and it is the subject of this chapter.

The coarsening of a new phase is generally well understood for vanishingly small initial supersaturations (characterized by a dimensionless parameter $\Delta_0 \ll 1$ which has to be defined appropriately) as long as only one length scale, the size of the particles R , is relevant in the system. In this case the distance between the different precipitates is large and a mean field theory in the sense of Lifshitz, Slyozov and Wagner [47, 78] is applicable.

In the previous chapter we studied the coarsening of melt inclusions inside an overheated

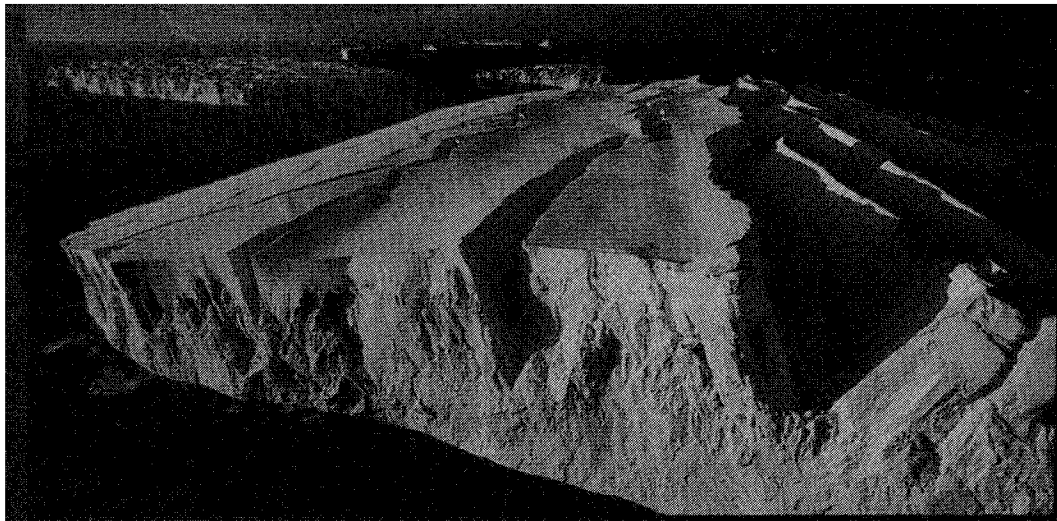


Figure 5.1: Strong interactions of neighboring cracks can happen even in geological formations. The overall stress relaxes in a coarsening process.

crystal. The scenario depicted there behaves crucially different from the classical coarsening theory. We pointed out that in this situation the assumption of a single relevant length-scale existing in the system cannot hold. The density difference of the two phases causes noticeable elastic deformations of the surrounding crystal. As a consequence the precipitates are not spherical but crack-like inclusions with a height $h \ll R$. It turns out that this is incompatible with the mean field requirement that different inclusions stay remote from each other, even in the limit of a vanishingly small overheating Δ_0 . Strong interactions between adjacent inclusions alter the growth laws and lead to nontrivial predictions. The Griffith condition plays a central role and gives a strong hint towards a closer connection between the theory of first order phase transitions and the theory of fracture.

The main aim of this chapter is to analyze the coarsening of cracks in uniaxially strained solids. We emphasize that this process is not accompanied by a real phase transition and it is very much different from the one discussed in [10]. However, the strong analogy between crack-like inclusions in melting processes and real cracks in a stressed solid still holds. Since the lateral extent of the cracks is much bigger than their opening, they come close to each other during the coarsening stage. This limit has so far been almost inaccessible to analytic and numerical calculations, and therefore it is quite remarkable that a derivation of the scaling laws is possible.

In the next section, which is the main part of this chapter, we derive the scaling laws for the collective fracture process in a uniaxially strained solid. We discuss the obtained results in section 5.3 and compare them to the coarsening process in the previous chapter. Though for an irregular arrangement of cracks only a derivation of the scaling laws for the average quantities is possible, an exact solution of the elastic problem can be found for a regular layer structure of cracks. It is presented in section 5.4.

This chapter is published in [11].

5.2 The uniaxially strained solid

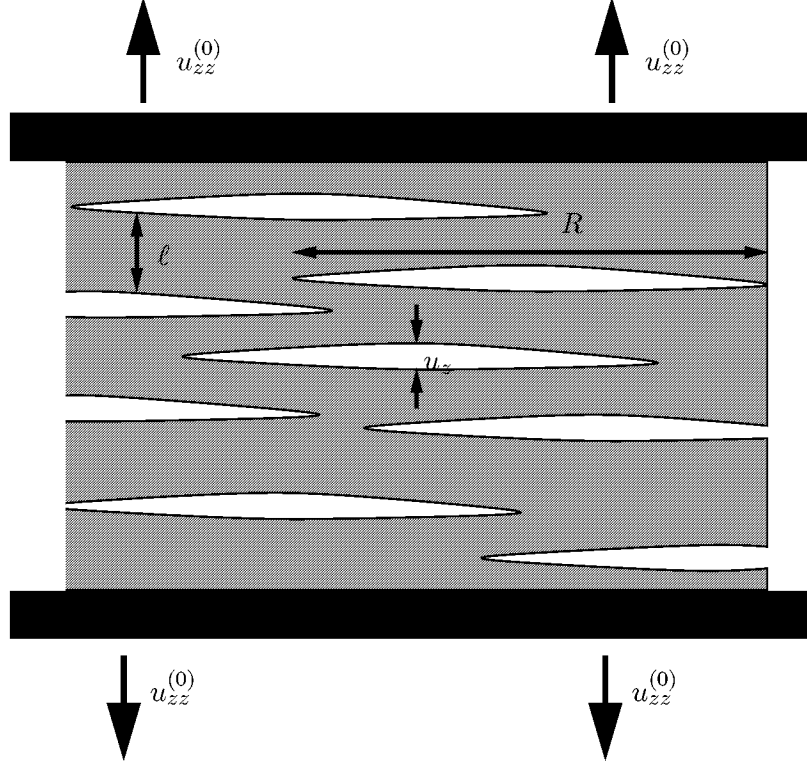


Figure 5.2: An infinitely large block of solid is fixed between two pistons (black). Initially no cracks exist in the system and a homogeneous strain $u_{zz}^{(0)}$ is present everywhere.

If a uniform isotropic tension is applied at infinity, all crack orientations are present with the same probability and the approach between several of them finally leads to the formation of a crack network [46, 38]. If, on the other hand, we stretch a block of a perfect solid in only one direction (which we call the z -direction) and then fix it in this position that a uniform strain $u_{zz}^{(0)}$ is maintained in the solid (see Fig. 5.2), then the situation is different. Our goal is to describe the time evolution in this arrangement.

Obviously the initial uncracked configuration is far from equilibrium: a high elastic energy density $w_{el}^{(0)} \sim E u_{zz}^{(0)2}$ could be dramatically reduced through the appearance of cracks in the system (E is the Young modulus). Finally, if only one long crack traverses the whole block, the system is completely unstretched and only a small amount of surface energy remains due to the two new crack surfaces. Refraining from these finite size effects we assume that a statistical ensemble of cracks appears in the solid with a growing mean size similar to the coarsening during a phase transition.

These cracks are mainly aligned perpendicular to the z axis because this maximizes the elastic energy release rate. Apart from the average size of the cracks R we introduce another length scale ℓ , which is the characteristic vertical distance between them. Only the assumption $\ell \ll R$ leads to consistent predictions. One can easily understand that a single (macroscopic) length scale L is not sufficient: In this case the spacing between neighboring cracks would be of

the same order L as the cracks themselves, and thus they would be almost independent. From dimensional reasons the average crack opening would be of order $u \sim PL/E$ and the strain would be $u_{zz}^{(0)} \sim u/L$. Hence the average stress would remain almost constant $P \sim Eu_{zz}^{(0)}$. Under these circumstances the system can never reach its equilibrium configuration with $P = 0$ and therefore the assumption of only one relevant length scale cannot be correct. In the following we will restrict our calculations to some simple order-of-magnitude estimates, assuming that the length scales of the system obey the order relation $R \gg \ell \gg u_z$; later we will see that these assumptions are self-consistent.

In the late stage of the coarsening process the main displacement comes from opening of the cracks and not from stretching. Thus

$$u_{zz}^{(0)} \sim \frac{u_z}{\ell}, \quad (5.1)$$

where we denote the average opening of the cracks by u_z . This equation corresponds to the global conservation law of conventional Ostwald ripening when almost all excess heat of the initially overheated system is converted to latent heat in order to perform the phase transition. The strain $u_{zz}^{(0)}$ in Eq. (5.1) corresponds to the supersaturation parameter Δ_0 mentioned above.

The distribution of cracks throughout the solid is irregular. It means that all of them are nearly perfectly aligned but the spatial distribution is random. The shape of the different cracks is not unique either. Because of these reasons an exact solution of the elastic problem is not possible. However, simple, basically dimensional, arguments of the theory of thin plates allow us to derive the desired scaling behavior. First of all, let us present this scaling description, and then we will enlighten the elastic problem more carefully giving an exact two-dimensional calculation in the case of a regular arrangement of cracks.

The solid between two neighboring cracks in vertical direction can be understood as a thin circular disk of lateral extent R and height ℓ . Its top and bottom are free surfaces with boundary conditions $\sigma_{zz} = \sigma_{rz} = 0$. At the tips of the cracks three (or more) of those plates come together and exert forces and torques on each other. These forces produce an average stress $P \sim \sigma_{zz}$ in the plates, which causes a bending of them. Bending of thin plates subject to a stress P is described by the fourth-order equation (see section 2.9)

$$\frac{E\ell^3}{12(1-\nu^2)}\Delta^2 u_z = P. \quad (5.2)$$

Here $\Delta = \partial_x^2 + \partial_y^2$ is the two dimensional Laplacian; ν and E are the Poisson and Young coefficients respectively. From this equation it follows readily that an average stress P is related to the opening u_z by

$$u_z \sim P \frac{1-\nu^2}{E\ell^3} R^4. \quad (5.3)$$

The corresponding deformation volume (the volume of the void inside the crack) behaves like

$$V \sim P \frac{1-\nu^2}{E\ell^3} R^6 \quad (5.4)$$

and the related release of the elastic energy per plate is

$$W_{el} \sim -PV \sim -P^2 \frac{1-\nu^2}{E\ell^3} R^6. \quad (5.5)$$

On the other hand the growth of the cracks is accompanied by an increase of surface energy

$$W_s \sim \alpha R^2 \quad (5.6)$$

with α being the surface tension.

Near the crack tips the theory of thin plates breaks down and stresses exhibit the typical $\sigma \sim r^{-1/2}$ -behavior at distances $r \ll \ell$ from the tip. Local equilibrium requires an additional variation of the total energy $W = W_s + W_{el}$ with respect to R . This results in a relation between the length scales and the stress in the system:

$$R \sim \frac{E\alpha}{1-\nu^2} \frac{1}{P^2} \left(\frac{\ell}{R} \right)^3. \quad (5.7)$$

It is a generalization of the Griffith condition for a single crack which can be retained by setting $\ell \sim R$ on the right hand side. Eq. (5.7) gives the critical size: bigger cracks grow and smaller ones shrink.

Another equation to determine the three unknowns R , ℓ and P follows from the conservation law (5.1) in combination with (5.3):

$$P \sim u_{zz}^{(0)} \frac{E}{1-\nu^2} \frac{\ell^4}{R^4}. \quad (5.8)$$

One of the most important differences to usual Ostwald ripening is the lack of a conserved order parameter. In the case of crack propagation, dissipation predominantly takes place in the close vicinity of the tips and diffusional transport of vacancies through the bulk is not required. Therefore kinetics of this mechanism is relatively fast and is commonly described by the phenomenological equation

$$R\dot{R} = -\kappa \frac{dW}{dR} \sim \kappa \left(P^2 \frac{1-\nu^2}{E\ell^3} R^5 - \alpha R \right). \quad (5.9)$$

Here κ is the kinetic coefficient that relates the energy release rate to the tip velocity. It contains information about small scale physics in the vicinity of the tip of the propagating crack. The combination $\Gamma(\dot{R}) = \alpha + \dot{R}/\kappa$ is the so-called fracture energy that is different from the ordinary surface energy α since it contains also the dissipation term $\dot{R}/\kappa$. The additional factor R in Eq. (5.9) appears due to the use of polar coordinates to describe growth of an almost circular crack. Notice that the relation (5.9) holds only for relatively low propagation velocities, as it is the case here in this problem. For higher velocities inertial terms have to be taken into account and the velocity is limited by the Rayleigh speed. Then also a tip-splitting can happen and the velocity starts to oscillate. We will study this regime in chapter 6.

Because of the Griffith (5.7) condition, both energy contributions in Eq. (5.9) are of the same order and one immediately obtains

$$R \sim \alpha \kappa t. \quad (5.10)$$

Also, combining Eqs. (5.7) and (5.8), we find

$$\ell \sim \left(\frac{E}{1-\nu^2} \right)^{-1/5} \alpha u_{zz}^{(0)-2/5} (\kappa t)^{4/5}. \quad (5.11)$$

Thus the average stress indeed decreases to zero like

$$P \sim \left(\frac{E}{1 - \nu^2} \right)^{1/5} u_{zz}^{(0)-3/5} (\kappa t)^{-4/5}. \quad (5.12)$$

The preceding three formulas are the main results of this chapter. They undoubtedly show the transition to equilibrium, i.e. the decrease of the stress and the growth of the length scales. From Eq. (5.1) it follows readily that the condition $u_z \ll \ell \ll R$ is clearly fulfilled, provided that $u_{zz}^{(0)} \ll 1$. This justifies the application of the theory of thin plates self-consistently.

5.3 Discussion

We point out that the growth law (5.10) is quite remarkable in some ways. It describes the growth with a constant velocity $v \sim \alpha\kappa$. In comparison, in usual cases of Ostwald ripening the transition to equilibrium happens with a decaying velocity, $R \sim t^\beta$ with $\beta < 1$ [47, 78, 10], and the process becomes slower and slower. The obtained scaling $R \sim t$ is probably the fastest growth law which is possible in dissipative systems. It is also noticeably that the velocity v is completely determined by material parameters and does not depend on the “supersaturation parameter” $u_{zz}^{(0)}$. Hence there is no reason for this velocity to be tuneably small. If however the material excels by a high robustness against fracturing, characterized by a small κ , this velocity can be smaller than the speed of sound and below the branching threshold [65], since the stress relaxes with time and the characteristic size of cracks maintains near the Griffith size (5.7). In this case, firstly, the used static approximation of the theory of elasticity is legitimate; and secondly, it is even conceivable to observe the process described here in small-scale laboratory experiments, provided that still a statistical ensemble of cracks is present. Otherwise the system can break into pieces by the very fast growth of one single or only a few cracks. For higher velocities it should still be possible to observe the statistical behavior in geological systems which can extend over kilometers (see Fig. 5.1).

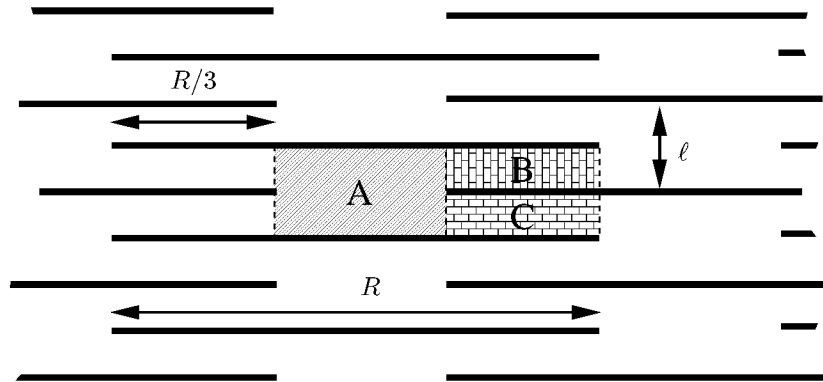


Figure 5.3: Cross section through the solid with perfectly aligned cracks (solid lines). In this regular structure all cracks have exactly the same length R , their horizontal overlap is $R/3$ and their distance ℓ . The system consists (periodically continued) of three different plate types denoted by A, B and C.

One of the central ingredients of our theory is the Griffith condition (5.7). Local equilibrium requires the possibility of a retraction of subcritical cracks.

Under some circumstances this process might be forbidden or hampered by oxidation of the surfaces. Then we expect small cracks to remain in the system, even if they are subcritical. Nevertheless, they do not influence the scaling behavior. Indeed, inside a plate between two large cracks the horizontal stress is much bigger than its vertical component $\sigma_{zz} \sim P$. We estimate $\sigma_{rr} \sim E\ell\partial_R^2 u_z \sim PR^2/\ell^2$. If such a big plate is horizontally cut by much smaller cracks, the arising “microplates” are mainly stretched or compressed in horizontal direction and consequently hardly bent. We conclude that almost the whole opening comes from the big growing cracks which therefore characterize the coarsening. Nevertheless, the full hierarchy of length scales remains in the system, hence exhibiting a fractal behavior. It turns out that the surface energy of the smallest “frozen” cracks of length L , which are still remote from each other, contain nearly the whole surface energy density $w_s \sim W_s/L^3 \sim \alpha/L$ which is proportional to the initial elastic energy density $w_{el}^{(0)} \sim Eu_{zz}^{(0)2}$. The rest dissipates and leads to a small increase of the temperature.

Finally, we emphasize that the growth law (5.9) is a phenomenological growth law which relates the propagation velocity to the energy dissipation rate. It is usually well fulfilled for relatively low propagation velocities. The aim of the next chapter is to gain a deeper understanding about possible kinetics in the crack tip region which allow a more sophisticated prediction of the crack growth speed.

5.4 Solution of the elastic problem for a regular arrangement of cracks

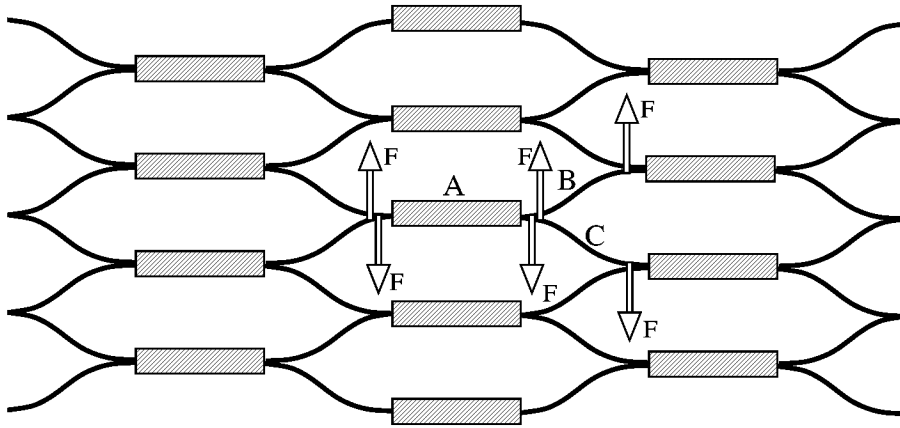


Figure 5.4: Schematic picture of the elastic situation in the perfectly regular structure. The thicker plate A is unbent, whereas forces F deform the plates B and C (solid lines). At each triple junction of plates the total force and torque are zero. The vertical string of B/C plates forms a network of springs, horizontally connected through ‘A’s.

In the remaining part of this chapter we illuminate the elastic situation more carefully. In order to make analytical progress, we consider a two-dimensional solid with cuts inside as a basis. These cuts are chosen to be perfectly aligned as depicted in Fig. 5.3, all of them having

the same length R . If we neglect irregularities, this configuration of course does not lead to a coarsening, but since we are basically interested in the analysis of the elastic properties, we disregard this problem here. Since the horizontal distance is also of order R , we prescribe the horizontal overlap between the cracks to be $R/3$ without loss of generality. Obviously three different regions of the solid between neighboring cracks appear, denoted by letters A, B and C. The array of B and C plates forms a network of springs in vertical direction; horizontally they are connected through the thicker A plates. We already mentioned this interpretation in the previous chapter. Application of an external strain $u_{zz}^{(0)}$ bends the rods differently. From the symmetry present in this special arrangement it readily follows that B and C bend exactly the same but in opposite directions; A remains unbent (Fig. 5.4). Therefore it is sufficient to consider part B. At its bottom and top it is bounded by stress free surfaces, thus the right hand side of Eq. (5.2) vanishes and it reads $u_z(x)'''' = 0$. Choosing the origin $x = 0$ to be in the middle of B, i.e. $-R/6 < x < R/6$, symmetry allows only the general solution $u_z = ax^3 + bx$. It also requires the conditions $u'_z(\pm R/6) = 0$ to allow the periodic continuation in x -direction. To produce the average strain $u_{zz}^{(0)}$, the opening of each crack is determined by the condition $u_{zz}^{(0)}\ell/2 = 2u_z(R/6)$. Therefore the missing coefficients are $a = -27u_{zz}^{(0)}\ell/R^3$ and $b = 9u_{zz}^{(0)}\ell/4R$.

To maintain this shape point forces and torques must appear at the edge of the plate. The sum of them is zero at each triple junction of plates as one can easily see from Fig. 5.4. These forces are given by [42]

$$F = -\frac{E(\ell/2)^3}{12(1-\nu^2)}u_z'''(\pm R/6) = \frac{27E}{16(1-\nu^2)}u_{zz}^{(0)}\frac{\ell^4}{R^3}. \quad (5.13)$$

The average stress in the system is therefore $P \sim F/R$ which is exactly the relation (5.8).

5.5 Summary

In this chapter we studied the evolution of a uniaxially strained solid. Since it is far from its thermodynamical equilibrium, an arrangement of cracks with perpendicular orientation towards the applied force appears and coarsens in time until the system reaches its final state: being broken in pieces by a single crack which traverses the whole solid block.

This process is very similar to the coarsening process in the previous chapter, which underlines a deeper connection between first order phase transitions and fracture mechanics, not only in the initial stage, where a critical nucleus corresponds to a Griffith crack.

We derived a consistent set of scaling laws for the coarsening regime of this collective fracture process and obtained a linear growth law for the average crack length, $R \sim t$. For the vertical distance between neighboring cracks we received $\ell \sim t^{4/5}$, whereas the average stress in the system decreases like $P \sim t^{-4/5}$.

We related the energy release rate to the crack propagation velocity by a linear phenomenological law which is experimentally justified for low velocities as they appear here. In the next chapter we introduce a new theoretical model of crack growth which predicts also the more complicated behavior for higher dissipation rates.

Chapter 6

Fast crack propagation by surface diffusion

6.1 Introduction

One of the most challenging puzzles in nonequilibrium physics and materials science is the phenomenon of fracture. It is important for the vast field of material failure and probably also for friction processes [30]. Despite its relevance even the motion of a single crack is poorly understood [36]. Experimentally, the maximum attained crack velocities are far lower than the theoretically expected Rayleigh speed [27]. Beyond a critical velocity, a so far unpredictable tip splitting of the crack can occur, producing strange oscillations of the crack speed (see Fig. 6.1 and 6.2) [65].

In experiments the surfaces of a crack are often rough [5]. Some of these results are interpreted in the framework of models of cracks propagating in heterogeneous media. The other possibility for the roughening of the crack surfaces is the instability of the straight motion of the crack tip. Recent experiments revealed that many puzzling phenomena in brittle fracture are related to an oscillatory instability at velocities appreciably below the Rayleigh speed [24, 25, 6, 66]. There were several attempts in literature to investigate the stability of a propagating crack. The linear stability analysis of the quasistatic crack subject to mode *I* loading (opening mode, i. e. a tensile force is applied to the solid, perpendicular to the crack) has been performed by Cotterell and Rice [20] with subsequent refinement by Adda-Bedia and Ben Amar [2]. They employ the Griffith theory and the so called principle of local symmetry, i. e. the condition that the mode *II* (sliding mode) stress intensity factor K_{II} vanishes at the tip of the crack. Mode *II* means that the surfaces of the crack are sheared against each other by the influence of external forces. They found that the straight motion of the crack becomes unstable if the tangential loading exceeds a critical value.

The classical theories [27] are based on the linear theory of elasticity and on an integral energy balance in the vicinity of an infinitely sharp crack tip. However, a more detailed approach based on equations of motion for the crack shape is needed to describe the intriguing spectrum of phenomena near the crack tip. A crack cannot have a sharp tip but must be “blunt” - otherwise stresses would diverge at least in the framework of a linear theory of elasticity. Hence, the curvature of the crack tip is required as a new relevant dynamical variable which allows to avoid stress singularities. We emphasize that, in contrast to models which describe crack propagation by bond breaking at the infinitely sharp tip, growth with a

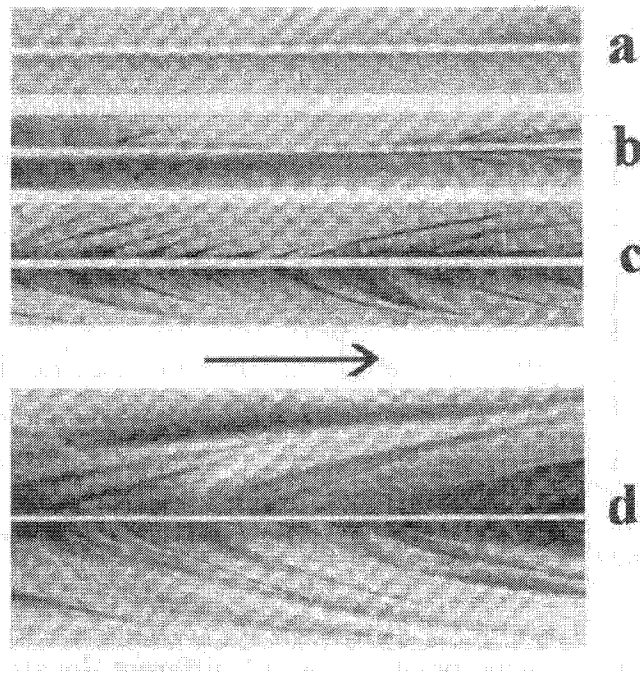


Figure 6.1: Crack growth in a narrow strip. For low propagation velocities, the cracks are straight, for higher velocities a tip splitting can occur [66]. In (a) the crack propagates with a speed below the threshold and is straight, in (b) the critical value is exceeded; small sidebranches appear. They become denser for higher velocities (c-d).

finite tip radius always requires a transport mechanism in order to preserve the shape (see Fig. 6.9). Recently it was proposed that this lengthscale is dynamically selected by the threshold of plastic deformations in the tip region [44]. Unfortunately, approaches of this type (see also [3, 39, 23, 27]) require the introduction of dynamic theories of plasticity which are usually much more speculative and less verified than the ordinary linear theory of elasticity.

In particular, a fully dynamical model, including the microscopic description of the cohesive zone around the crack tip, has been developed by Ching, Langer, and Nakanishi [18, 17]. The cohesive force in the neighborhood of the tip provides a fracture energy and a mechanism for regularizing the stress singularity; this model removes the need to speculate about a principle of local symmetry. In addition to Refs. [20, 2], they found a strong microscopic instability even for very low crack velocities, which depends very sensitively on tiny details of the cohesive-zone model. However, later Langer and Lobkovsky [45] showed that these cohesive-zone models in the framework of a sharp-tip representation lead to unphysical and unreasonable features of the elastic stresses in spite of a regularization by cohesive forces.

Here we demonstrate that the *linear theory of elasticity* is sufficient to describe consistently crack propagation, the necessary transport mechanism near the crack tip being *surface diffusion* along the crack surfaces. Of course, in many situations plasticity may be very important, but the beauty of our approach is that it predicts, in a simple and well controlled continuum theory, steady state crack growth, the tip splitting instability and also slow deformations of already existing cracks. The goal of this chapter is to present a completely new description of crack propagation by a *consistent* set of equations of motion. We focus our

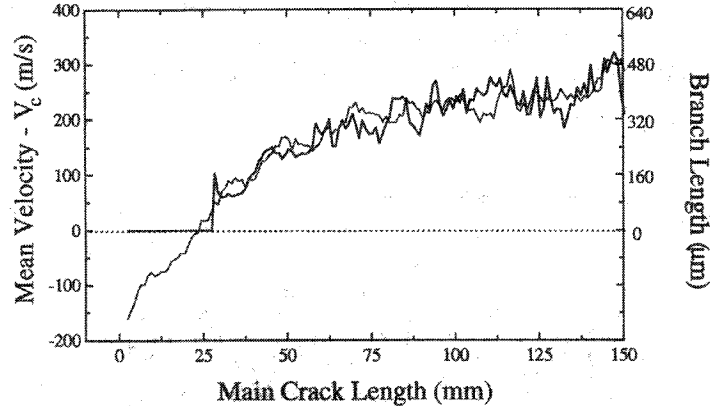


Figure 6.2: The propagation velocity starts to oscillate when a critical velocity is exceeded. The terminal velocity is appreciable below the Rayleigh speed [66].

interest on the generic features and qualitative predictions of this approach. Usually, many complicated inelastic processes happen in a zone around the crack tip. If one assumes that this process zone is relatively thin, then one can try to describe mass transport phenomena *effectively* by surface diffusion.

The idea of crack propagation by surface diffusion has previously been studied by Stevens and Dutton [74], who assumed an ad hoc crack shape which is not found by solving the full free boundary problem and requires mass transport over large scales. Therefore, their model cannot describe the usual fast crack growth.

Our basic mechanism is related to the Asaro-Tiller-Grinfeld (ATG) instability [4, 35], which predicts a morphological instability of a uniaxially stressed solid interface due to surface diffusion. Relatively long-wave perturbations of the interface lead to a reduction of the elastic energy of the system, whereas short-wave corrugations are hampered by surface energy. In the long time behavior, deep grooves can form, producing shapes similar to cracks [81, 72]. According to previous theories, which used only the *static* theory of elasticity, the notches propagate with increasing velocity and decreasing tip radius and collapse within finite time to a cusp singularity (see section 2.8.4). Similar to crack dynamics the lack of a tip radius selection becomes obvious, and already shows the close relationship between the ATG instability and crack propagation.

Usually, it is believed that surface diffusion is slow, but, surprisingly enough, it should not be ignored even in fast fracture processes. Our main idea is that surface diffusion is driven by the strong gradient of the chemical potential in the tip region. This can be a very efficient mechanism for crack propagation if the relevant transport length is sufficiently small. Additionally, energy release and strong dissipation bring the local temperature close to the melting temperature [28, 26]. This drastically increases the surface diffusion coefficient and makes fast crack propagation essentially independent of the outside temperature.

Section 6.2 presents some basic ideas to motivate the further steps: The cusp singularity of the Grinfeld instability and the arising difficulties are explained. Also it will be shown that Grinfeld instability and crack dynamics are related in a very special sense: It is shown

that the surfaces of an already existing crack are unstable and corrugate slowly. Afterwards, we argue that this instability can also be expected in the tiny tip region; we suspect that it might be responsible for a tip-splitting.

Section 6.3 is the main part of this chapter. Using simple and robust scaling arguments we explain the origin of the cusp singularity, and how it can be cured. This allows propagation of a notch with finite velocity; conversely, it can be interpreted as steady state growth of a crack by surface diffusion. For a local model of stresses we solve the equations of motion and obtain crack shape, propagation velocity and finite tip radius as function of the applied driving force. We argue that such a crack becomes unstable against a secondary Grinfeld instability, provided that a critical driving force is exceeded. This gives a completely new approach to understand a broad range of intriguing phenomena in fracture mechanics.

Main parts of this chapter are published in [12] and partly in [71].

6.2 Motivation

It is the intention of this chapter to elucidate the idea that a crack can grow by surface diffusion. Finally, it turns out that only a few ingredients are necessary for a self-consistent description: the linear theory of dynamic elasticity and the law of surface diffusion; both are well established elements.

We already mentioned a deeper link between fracture mechanics and the Grinfeld instability. Especially, if one looks at the deep grooves which can form in the late stage of the instability (see Fig. 2.9), it is quite natural to think about the most advanced notches as “cracks”. Also from an energetic point of view, both processes are similar: According to the Griffith theory, growth or shrinkage of a crack is determined by a competition of elastic and surface energy — the same is true for the Grinfeld instability. The main lack of the usual descriptions of crack propagation is that they do not provide a detailed equation of motion for the individual points of the crack tip which is no longer assumed to be atomically sharp. On the other hand, the Grinfeld instability has the advantage of a well defined equation of motion of surface diffusion, driven by a chemical potential. However, we already saw in section 2.8.4 that the Grinfeld instability ends up in an unphysical singularity after finite time; the tip radius becomes zero and the propagation velocity diverges.

It is one of the main goals of this chapter, firstly to understand the origin of this singularity and, secondly, to overcome it. Then it can provide a mechanism to explain crack propagation by surface diffusion, since indeed the notches of the Grinfeld instability behave in the same way as a crack.

In the following section we demonstrate the collapse to the finite time singularity. Though we do not solve the problem here, we speculate about the influence of a “secondary Grinfeld instability” on the motion of a crack. At first, we discuss briefly its relevance to the surfaces of an already existing crack in section 6.2.2. There we introduce certain scaling arguments, which can afterwards also be applied to a localized instability in the tip region. This is done in section 6.2.3.

6.2.1 The cusp singularity

Later in this chapter we will derive that the cusp singularity is a very generic feature of the Grinfeld instability. It happens, because the governing equations do not provide a lengthscale selection for a tip radius. In this sense, it is present not only in Grinfeld instability processes

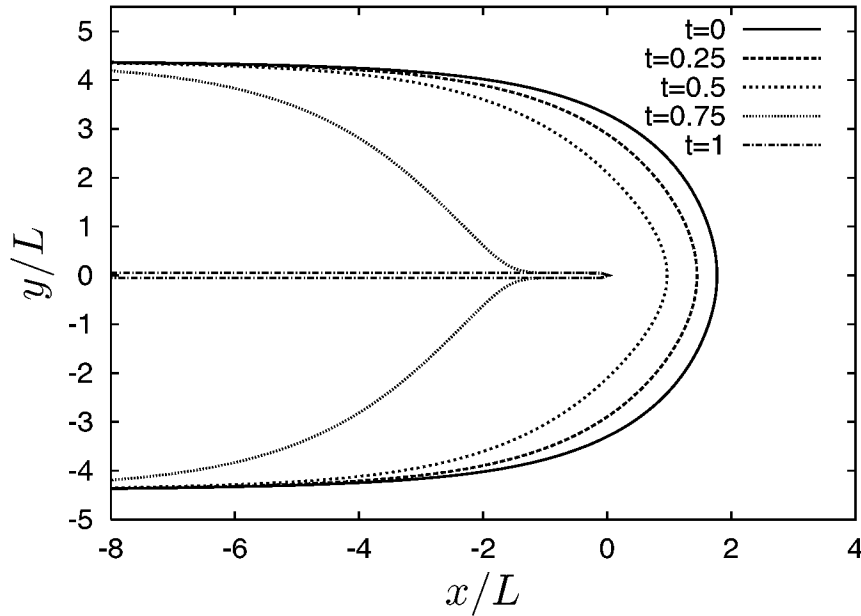


Figure 6.3: Evolution of an initial shape without inertial effects in a co-moving frame of reference. The tip radius decreases and the cusp singularity is cut off only by the grid resolution. An intrinsic lengthscale is not present in this problem, therefore the shape is given on the arbitrary lengthscale L . The unit of time is L^2/D_{mc} with the diffusion constant D_{mc} . Details are explained in chapter 7.4.

which are driven by surface diffusion, but also for a solid which is in contact with its melt. Here a melting and recrystallization leads to the formation of the same deep grooves. The finite time singularity has been observed in many analytical and numerical simulations (see e.g. [40, 19] and references therein). It is generic in the sense that it depends only on very few properties of the elastic fields in the vicinity of the tip.

Later in this chapter, we will introduce a local model of stresses (see section 6.3.2) which reflects all important features of the real stress field. At the moment, we refrain from introducing this model here. In Fig. 6.3 the evolution of a “finger” is shown; the underlying kinetics is melting and recrystallization. The employed numerical methods to calculate the time evolution of this process will be explained in chapter 7.3. Here we demonstrate only the collapse to the singularity: An initial “crack” with finite tip radius becomes sharper and sharper until it reaches the numerical discretization. Simultaneously, the propagation velocity increases and the tip radius decays. Details will be given later in chapter 7.4.

6.2.2 Grinfeld instability on crack surfaces

In this section we start to explain the idea how fracture mechanics and Grinfeld instability belong together. We demonstrate that the conditions for the occurrence of the latter instability, nonhydrostatic stresses at the surface, are fulfilled on the cut lines of a straight crack. This leads to a reshuffling of material along the already existing crack shape, but cannot be responsible for instabilities of a fast moving crack tip. It introduces the important idea of

a “quantization” of the instability by boundary conditions which leads to a criterion for the appearance of an instability; this concept will also be used later for instabilities of the crack tip itself. Here we refrain from a complete derivation of the results, which are presented in [70] and published, together with later extensions, in [71].

In all conventional descriptions a crack is recognized as the trace left behind the propagating crack tip. In this sense its surfaces are “frozen” and not subject to any additional dynamics. However, we realized that on the surfaces of a straight crack which is subjected to a remote tensile stress P , the normal stresses are zero, $\sigma_{nn} = 0$, but the tangential stresses do not vanish, $\sigma_{\tau\tau} = -P$ [8, 71]. Therefore, the Grinfeld instability can occur and deform the crack even behind the tip; slight deformations of the crack shape can reduce the total energy of the system.

At this stage, we ignore for the moment the complicated dynamics in the tip region and describe a crack by a mathematical cut between the end points $x = \pm L$ on the y axis (see Fig. 6.4). We compare the energy of a straight crack, described by $y_0(x) \equiv 0$ to the energy of a

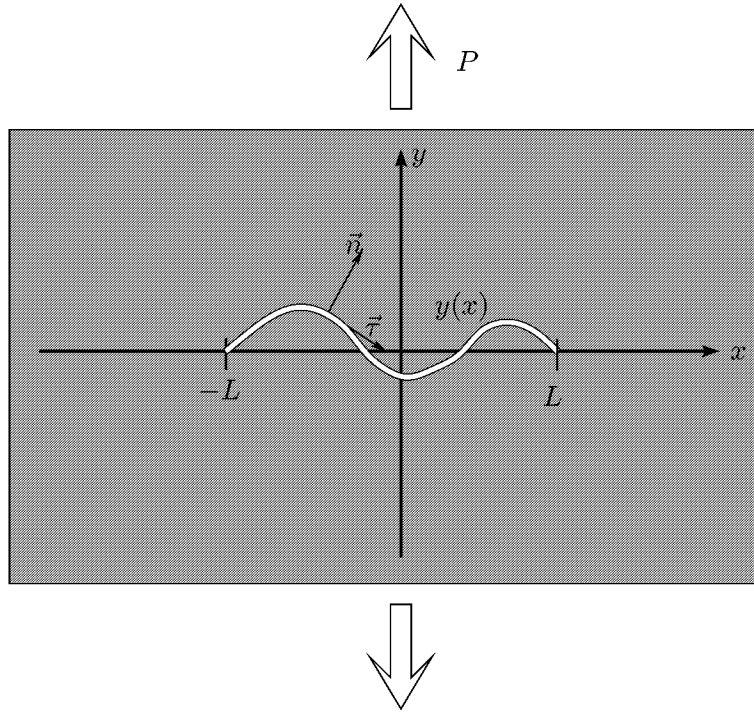


Figure 6.4: An originally straight crack in a two-dimensional solid with end points $\pm L$ can deform to a wavy shape due to the Grinfeld instability if a tensile load P is applied far away to the solid.

wavy crack $y(x)$ to lowest order in this perturbation. All dynamics of the tips are suppressed, thus we keep the points $y(\pm L) = 0$ fixed. Similarly to section 2.8, the perturbation decreases the elastic energy but increases the surface energy. Due to the “quantization” by the fixed end points, the straight crack is only unstable with respect to morphological deformations, if the characteristic wavelength of the instability fits into the interval $[-L : L]$. Since the Grinfeld length is of order of the Griffith length, the instability can only develop if the crack length is itself of order of the Griffith length L_G . A detailed numerical analysis [71] shows

that the instability occurs if the crack length L exceeds the critical value $L_c = 5.18 L_G$. The complete and rather technical calculations together with their numerical evaluations clearly prove the mentioned interpretation that the characteristic wave length has to fit into the “quantization” interval $2L$. Indeed, this leads to a discrete set of eigenmodes which fulfill the boundary conditions. If we assign the energy $U = 0$ to the straight crack, then all perturbations lead to higher energies for $L < L_c$ (see Fig. 6.5). On the other hand, the crack becomes unstable if the energy of the lowest mode becomes negative; then a perturbation of the crack shape can reduce the total energy of the system. The eigenmode which belongs to

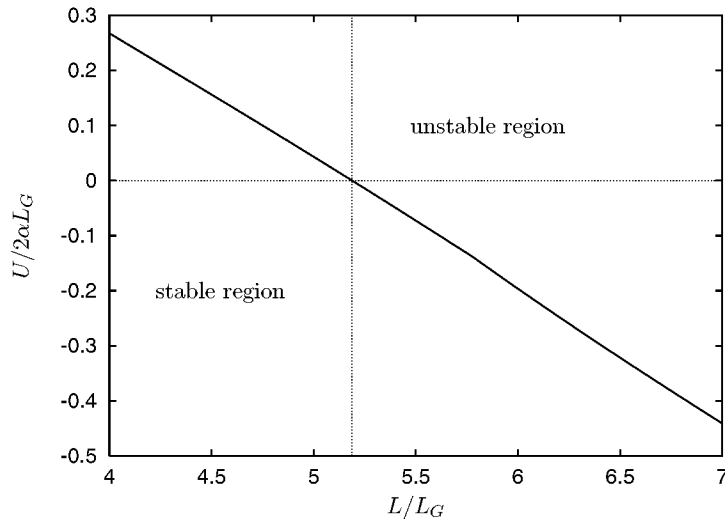


Figure 6.5: The normalized energy of the most unstable eigenmode of the Grinfeld instability on a crack as function of its length. As soon as it becomes negative, the system gets unstable.

a critical crack is depicted in Fig. 6.6. However, we remark that the instability occurs only in a regime where the crack itself wants to grow because the Griffith threshold is exceeded, i.e. $L > L_G$. Therefore the Grinfeld instability is quite likely convectively transported away from the crack tip, and the long-wave perturbations cannot be relevant for dynamical instabilities of the tip which lead to an irregular propagation or even a splitting of the tip. The reason is that we suppressed all degrees of freedom of the tip. The fact that the Grinfeld instability occurs only for propagating cracks (since $L_c > L_G$) makes it difficult to observe the effect experimentally.

To overcome this problem, the addition of a homogeneous remote tangential stress P_x as sketched in Fig. 6.7 can shift the threshold of instability. We declare P_x to be positive for a tensile stress and introduce the dimensionless parameter $\beta = P_x/P$. The critical length becomes a function of β as well; this dependence is plotted in Fig. 6.7. For $\beta = 0$ we retain the former result $L_c = 5.18 L_G$. The most interesting range is $0 < \beta < 1$: The pure tensile loading perpendicular to the crack causes a tangential stress $\sigma_{xx} = -P$ along a straight crack. The additional loading $P_x > 0$ reduces this value to $\sigma_0 = \sigma_{xx} = -P + P_x < 0$ and thus hampers the evolution of the Grinfeld instability. Therefore the critical length increases in comparison to $\beta = 0$. For $\beta \rightarrow 1$ the nonhydrostaticity vanishes completely and the Grinfeld instability cannot occur. Consequently the critical length diverges. In other words, the change of the elastic energy during redistribution of matter is at least of order $\mathcal{O}(y^4)$ in the deviation

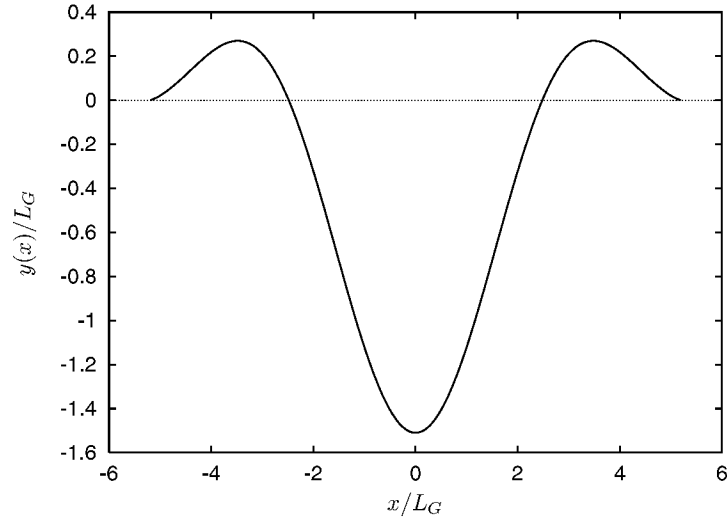


Figure 6.6: Universal shape of the critical crack, $L = 5.1882 L_G$. The energy of this crack is $U = 0$.

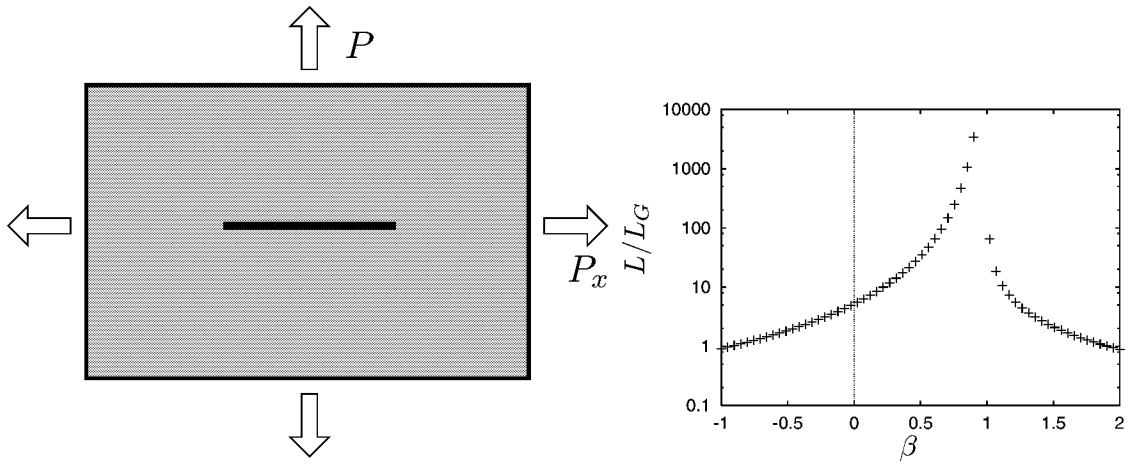


Figure 6.7: A crack in a solid which is subjected to a tensile stress P . By addition of a tangential stress P_x , the onset of the Grinfeld instability can be shifted. In the right graph, the dependence of the critical length on the loading ratio, $\beta = P_x/P$, is shown. For $P_x = 0$, we obtain the particular result $L_c = 5.18 L_G$.

from the straight line $y = 0$. This result has already been derived in [15].

For $\beta < 0$ the compressive surface stress is even increased and the critical length becomes smaller.

The case $\beta > 1$ means that the horizontal stress becomes bigger than the vertical loading. Generally, the elastic energy release $dU_{el}/dL \sim K_I^2 + K_{II}^2$ during crack relaxation is maximized if the crack orients perpendicular to the direction of the highest stress. A vertical orientation of the crack is forbidden by the boundary conditions $y(\pm L) = 0$; but by taking on a wavy shape the crack tries to mimic this optimal shape. This tendency becomes stronger with higher values of P_x . Therefore $L_c \rightarrow 0$ for $\beta \rightarrow \infty$.

6.2.3 The elliptical crack

In the previous section we demonstrated that the surfaces of a crack are subject to the Grinfeld instability even far away from the tip. Now immediately the question arises whether this effect can also appear in the tip region. Here we use similar scaling arguments to show that the Grinfeld instability can indeed also be expected in the tip region. We speculate that it can be responsible for a tip-splitting instability.

First we call to mind that it has not yet been shown that a crack-like structure which allows for surface diffusion can exist in a stable sense. So far, these cracks always seem to collapse to a finite-time singularity, and it still has to be cleared up why this problem occurs and how it can be solved. Nevertheless, in this section we want to assume that we have a “stable” crack. Our aim is to enlighten whether and why an instability in the tip region can take place.

We consider an elliptical hole in an infinite solid; in the framework of the static theory of elasticity, this problem can be solved analytically [54]. We model a crack as a limit of the ellipse with semiaxes a and b with $a \gg b$ (see Fig. 6.8).

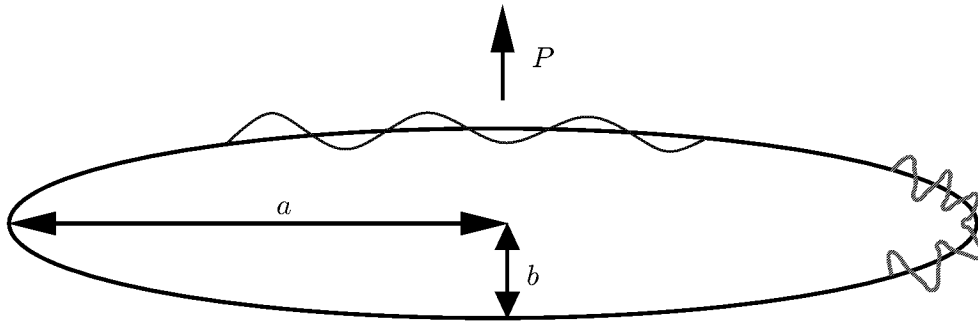


Figure 6.8: A solid with an elliptical hole which is subjected to an external pulling stress. Surface diffusion can lead to the long-wave instability along the flat part of the shape, but also in the narrow tip region.

The long-wave instability of the preceding section can occur if the crack length is of order of the Griffith length, i.e.¹

$$a \sim \frac{E\alpha}{P^2}. \quad (6.1)$$

¹We suppress the dimensionless Poisson ratio which does not affect the scaling behavior.

Then the characteristic wavelength of the instability fits into the “quantization interval” $2a$.

From the analytical solution, we obtain that the tangential stresses at the tip behave like

$$\sigma_{\tau\tau}^{(tip)} \sim Pa/b. \quad (6.2)$$

In agreement with the statement that stresses diverge at an infinitely sharp tip, this value tends to infinity in the limit $a/b \rightarrow \infty$.

The local Grinfeld length at the tip,

$$L_{Gr}^{(tip)} \sim \frac{E\alpha}{\sigma_{\tau\tau}^{(tip)^2}}, \quad (6.3)$$

has to be of the same order of the characteristic geometrical lengthscale, the tip radius

$$r^{(tip)} \sim b^2/a, \quad (6.4)$$

in order to allow the occurrence of the instability. This leads to the result

$$a \sim \frac{E\alpha}{P^2}. \quad (6.5)$$

Notice that the small lengthscale b has dropped out of this relation. The threshold of instability therefore depends only on the “macroscopic” parameters a and P ; in particular, the threshold of instability is again of order of the Griffith length, and therefore it is conceivable that this effect can become relevant for crack propagation processes. One can speculate that the corrugation of the shape is the onset of the tip splitting instability.

6.3 Fast crack growth by surface diffusion

In this section we derive why the Grinfeld instability must collapse to a finite time singularity. We show that this is due to the use of the *static* theory of elasticity, and that the arising problems can be cured by application of the full *dynamic* theory of linear elasticity. This also allows fast crack growth by surface diffusion. The underlying mechanism is explained in section 6.3.1. It results in a complicated *nonlinear, nonlocal multiscale elastodynamic free boundary problem* which cannot be easily solved. Therefore, in section 6.3.2, a local model for the stress field is introduced; we do not solve the elastic problem exactly but mimic stresses in a local way. This permits to calculate steady state motion of a crack tip for a given driving force Δ and also the dependence of the propagation velocity and the tip radius on Δ .

In section 6.3.3, we argue that a crack which advances by surface diffusion, is subject to a secondary Grinfeld instability, provided that the driving force exceeds a critical value. This leads to a tip-splitting of the crack.

We discuss the consequences of this model for crack propagation in section 6.3.4. The most important result is that *fast* growth by surface diffusion is indeed possible. And also, though it is a continuum theory not involving atomic properties, it turns out that the scale of the tip radius is indeed Ångström, in agreement with experimental observations.

In section 6.3.5 we discuss in more detail the implications of one of the main ingredients to our model, the linear theory of elasticity. We introduce the terms “referential” and “spatial” description, which are usually associated to elastic and hydrodynamic problems. However, in fracture mechanics where displacements can become large, one has to be more careful with the applications of the different descriptions.

6.3.1 Steady state crack growth

In this section we explain that fast crack propagation by surface diffusion is possible. By counting arguments it is shown that introduction of the dynamic theory of elasticity overcomes the cusp singularity of the Grinfeld instability. In turn, this allows steady state growth of a crack.

We use a two-dimensional plane-strain situation with mode I loading to describe crack propagation [27]. On the surfaces of the crack the normal stress σ_{nn} and the shear stress $\sigma_{n\tau}$ vanish, whereas the tangential stress $\sigma_{\tau\tau}$ usually does not. The chemical potential at the interface is given by (see chapter 2.8.2)

$$\mu = \Omega \left(\frac{1 - \nu^2}{2E} \sigma_{\tau\tau}^2 - \alpha \kappa \right). \quad (6.6)$$

Here α is the surface energy, κ the curvature of the interface and Ω the atomic volume. E and ν are Young's modulus and Poisson ratio, respectively. Non-hydrostatic stresses drive a surface flux proportional to the gradients of the chemical potential along the surface; in turn the normal velocity equals the divergence of this flux due to conservation of material,

$$v_n = - \frac{D}{\alpha \Omega} \frac{\partial^2 \mu}{\partial s^2}, \quad (6.7)$$

where $\partial/\partial s$ denotes the tangential derivative and D (dimension m^4s^{-1}) is proportional to the surface diffusion coefficient. (It is related to the usual surface diffusion coefficient D_s by $D = D_s \Omega^2 \delta \alpha / kT$. Here δ is the number of atoms per unit area of surface, k the Boltzmann constant and T the temperature.)

First, we are interested in steady state solutions of the equation of motion, with a crack moving in positive x -direction with velocity v (see Fig. 6.9); In co-moving polar coordinates, $x = r(\theta) \cos \theta$, $y = r(\theta) \sin \theta$, the steady state equation for the shape $r(\theta)$ reads after one integration of Eq. (6.7)

$$vr \sin \theta = - \frac{D}{\alpha \Omega} \frac{1}{\sqrt{r^2 + r'^2}} \frac{d\mu}{d\theta}. \quad (6.8)$$

The derivation of this equation is given in appendix A. Generally speaking, this, together with Eq. (6.6), is a complicated, non-linear third order equation with non-local contributions arising from the elastic fields, since $\sigma_{\tau\tau}$ depends on the entire shape.

In the tail region stresses decay and the shape equation is a third order linear differential equation $Dy''' = vy$ with two growing (and oscillating) and one decaying solution. Only the latter, $y(x \rightarrow -\infty) = A \exp[(v/D)^{1/3}x]$, asymptotically describes physical shapes and is allowed. Let us focus on symmetrical solutions, $r(\theta) = r(-\theta)$, and start integration at the crack tip $\theta = 0$. Since the physical properties, curvature and stresses, do not depend on the choice of coordinate system but only on the crack shape, we can arbitrarily choose $r(\theta = 0) = r_0$, with the a priori unknown tip radius $r_0 = 1/\kappa(0)$. Then from symmetry and the definition of the tip curvature, $\kappa = (r^2 + 2r'^2 - rr'')/(r^2 + r'^2)^{3/2}$, the natural conditions $r'(0) = r''(0) = 0$ arise. Integration over the upper interface $\theta > 0$ requires the suppression of two growing exponentials at the tail, which imposes two boundary conditions. For a given external loading, these conditions can be fulfilled by a proper selection of the tip radius r_0 and growth velocity v . By this argument the situation seems to be fully described. However, as we mentioned already earlier, the use of a *static* theory of elasticity does not allow a

selection of the tip radius. The reason is, that both contributions to the chemical potential, surface energy $\mu_s \sim \kappa$ and elastic energy $\mu_{el} \sim \sigma^2$, behave as r_0^{-1} close to the tip: In the tip approximation, stresses behave as [27] (see also chapter 2.6)

$$\sigma_{ij} = \frac{K}{r^{1/2}} f_{ij}(\theta) \quad (6.9)$$

with the static stress intensity factor $K \sim \sigma_\infty L^{1/2}$, where σ_∞ is the applied remote stress and L is the macroscopic length of the crack, $L \gg r_0$, which is not considered here. Instead we assume K to be kept fixed. The universal stress distribution f_{ij} depends only on the orientation relative to the crack [27]. The asymptotic distribution (6.9) is valid far away from the tip, $r_0 \ll r \ll L$, but it gives the correct scaling of stresses also on the crack surface $r \approx r_0$. Therefore, a dimensionless rescaling of all lengthscales, e.g. $\tilde{r} = r/r_0$, and of the growth velocity $\tilde{v} = vr_0^3/D$ leaves the equation of motion invariant and, thus, cannot determine the lengthscale r_0 . Consequently, a steady state solution does not exist. This is the reason for the already mentioned cusp singularity of the ATG instability.

The main idea of this chapter is based on the fact that a full *elastodynamic* description restores the selection of this lengthscale. It is known that at least for higher crack speeds the angular distribution f_{ij} become strongly dependent on the ratio v/v_R (v_R is the Rayleigh speed [27]). The dynamical stress intensity factor K_{dyn} is related to the static one used here by an extra velocity dependent function $g(v/v_R)$, $K_{dyn} = Kg(v/v_R)$. The crucial observation is, that velocity appears now in two different combinations in the equation of motion, vr_0^3/D and v/v_R . Thus, by introduction of the new parameter v/v_R , a selection of both v and r_0 happens.

From these general arguments we conclude that fast steady state crack propagation by surface diffusion is indeed possible. However, the exact solution of the problem is technically very difficult, because it requires the solution of an elastodynamic problem for an a priori unknown crack shape and also involves several very different length scales. For the moment we neglect the full dynamical modifications to Newton's equation, the boundary conditions and also to the chemical potential. We will study these effects later in section 7.1. They lead to the appearance of the parameter $(v/v_R)^2$ in the problem compared to the quasistatic description. Evaluation of the exact equations of motion requires extended numerics, especially in the time-dependent case.

6.3.2 The local crack tip model

Since we have seen in the previous section by application of counting arguments that crack growth by surface diffusion should be possible, we try now to exploit this idea. We simplify the problem in order to make further analytical progress and to expose the general idea of our approach. It will turn out that one cannot describe all effects by this approximation and further refinement is necessary, but the main results are qualitatively very robust against changes of the model. In particular, it allows to predict the tip radius, the propagation velocity and the shape of the crack as functions of the applied stress.

We mimic the tangential stress by a *local* description in the spirit of Eq. (6.9), as depending on the propagation velocity and only on the local properties of the interface. It takes both the velocity dependence of the angular distribution and the decrease of the dynamical stress

intensity factor into account:

$$\sigma_{\tau\tau} = K \left[\sqrt{1 - (v/v_R)^2 \cos(\theta/2)} + (v/v_R)^2 \sin^4 \theta \right] / r^{1/2}. \quad (6.10)$$

This form reflects the first order transition of the principal stress direction $\theta = 0$ for low velocities towards $\theta \neq 0$ as function of v/v_R [27]. The use of more sophisticated expressions (e.g. the singular dynamical field in full detail) would not provide a large gain, since, anyway local approximations cannot lead to exact results. For the same reasons we also neglect inertial corrections to the boundary conditions in and in the chemical potential (see chapter 7.1).

However, we have checked that a model with a continuous transition in azimuthal stress (replacement of $\sin^4 \theta$ by $\sin^2 \theta$ in Eq. 6.10) gives qualitatively the same results.

Now Eq. (6.8), together with (6.6) and (6.10), is a closed third order differential equation for the shape $r(\theta)$ which can be integrated numerically. In the tail region, a Cartesian representation of the shape $y = y(x)$ is most reasonable, whereas in the tip region we prefer a polar description, $r = r(\theta)$. At a suitable point, e.g. $x = -r_0$, both representations have to match.

The chemical potential (6.6) consists of an elastic and a surface contribution. We denote the elastic contribution by G ,

$$\mu = G(x) - \alpha\Omega\kappa \quad (6.11)$$

with

$$G = \Omega \frac{1 - \nu^2}{2E} \sigma_{\tau\tau}^2 \quad (6.12)$$

and

$$\kappa = -\frac{y''}{(1 + y'^2)^{3/2}} \quad (6.13)$$

in the Cartesian representation. We rewrite the steady state equation (see appendix A)

$$vy = \frac{1}{(1 + y'^2)^{1/2}} \frac{D}{\alpha\Omega} \frac{d\mu}{dx} \quad (6.14)$$

as a set of first order equations. The most convenient choice is to use the functions y , y' and μ as unknowns. Therefore we obtain

$$\frac{dy}{dx} = p, \quad (6.15)$$

$$\frac{dp}{dx} = -\frac{G - \mu}{\alpha\Omega} (1 + p^2)^{3/2}, \quad (6.16)$$

$$\frac{d\mu}{dx} = \frac{\alpha\Omega}{D} (1 + p^2)^{1/2} vy. \quad (6.17)$$

In the tail, the asymptotic behavior is given by

$$y = A \exp((v/D)^{1/3} x), \quad (6.18)$$

$$y' = A(v/D)^{1/3} \exp((v/D)^{1/3} x), \quad (6.19)$$

$$\mu = -\alpha\Omega\kappa = \alpha\Omega y'' = A\alpha\Omega(v/D)^{2/3} \exp((v/D)^{1/3} x). \quad (6.20)$$

The coefficient A is one of the shooting parameters of the problem. In the tip region, we have instead Eq. (6.8).

$$\kappa = \frac{r^2 + 2r'^2 - rr''}{(r^2 + r'^2)^{3/2}}. \quad (6.21)$$

The prime denotes the derivative with respect to θ . Then the set of first order equations for $r, p = r', \mu$ is

$$\frac{dr}{d\theta} = p, \quad (6.22)$$

$$\frac{dp}{d\theta} = \frac{r^2 + 2p^2 - (G - \mu)(r^2 + p^2)^{3/2}/\alpha\Omega}{r}, \quad (6.23)$$

$$\frac{d\mu}{d\theta} = -\frac{\alpha\Omega}{D}(r^2 + p^2)^{1/2}vr \sin \theta. \quad (6.24)$$

The tip curvature is $\kappa(0) = r_0^{-1}$. At the tip, $\theta = 0$, the boundary conditions are $r(\theta = 0) = r_0$, $r'(0) = 0$, $r''(0) = 0$. Therefore

$$\mu(\theta = 0) = G(\theta = 0) - \alpha\Omega r_0^{-1}. \quad (6.25)$$

At the intermediate matching point x_m , function values, slopes and the chemical potential have to have the same values from both sides of integration. This gives a set of shooting conditions. Since integration of the differential equations depends very sensitively on the parameters A, v and r_0 , they can be changed only very carefully in order to match the solutions. It turned out that instead of using Newton's method to fulfill e.g. $\mu(x_m^{(+)}) = \mu(x_m^{(-)})$, it is more robust to use a multi-dimensional simplex minimization routine [58] to minimize the expression

$$Res = (y^{(+)} - y^{(-)})^2 + (y'^{(+)} - y'^{(-)})^2 + (\mu^{(+)} - \mu^{(-)})^2. \quad (6.26)$$

This finally provides both the crack shape (Fig. 6.9) and a selection of v/v_R and r_0 as functions of the dimensionless driving force $\Delta = K^2(1 - \nu^2)/2E\alpha$. The results are given in Figures 6.10 and 6.11.

One of the main results is that the upper limit for the steady state crack velocity is appreciable below the Rayleigh speed, as known from experimental results. The instantaneous velocity in the non steady state regime can of course reach higher values [65, 26]. For relatively low driving forces, the growth velocity increases with increasing Δ , but for higher values of Δ , it even decreases. Simultaneously, the tip becomes sharper at first, but then blunts again.

6.3.3 Stability analysis

Here we give reasons for a morphological instability of the propagating crack tip. It can cause a tip splitting provided that a critical driving force is exceeded.

Although the decrease of the velocity v as function of Δ might be naively understood as a sign of instability, the model itself is stable: We performed a straightforward but tedious numerical stability analysis and found no unstable modes. The point is, that only v/v_R decreases, but vr_0^3/D increases. Only a decrease of this parameter, which appears in combination with the dissipative coefficient D , would be a real sign of instability.

Nevertheless, our solution is subject to the ATG instability above a critical threshold of the driving force Δ (see Fig. 6.12). The de-stabilizing effects stem from the non-local elastic

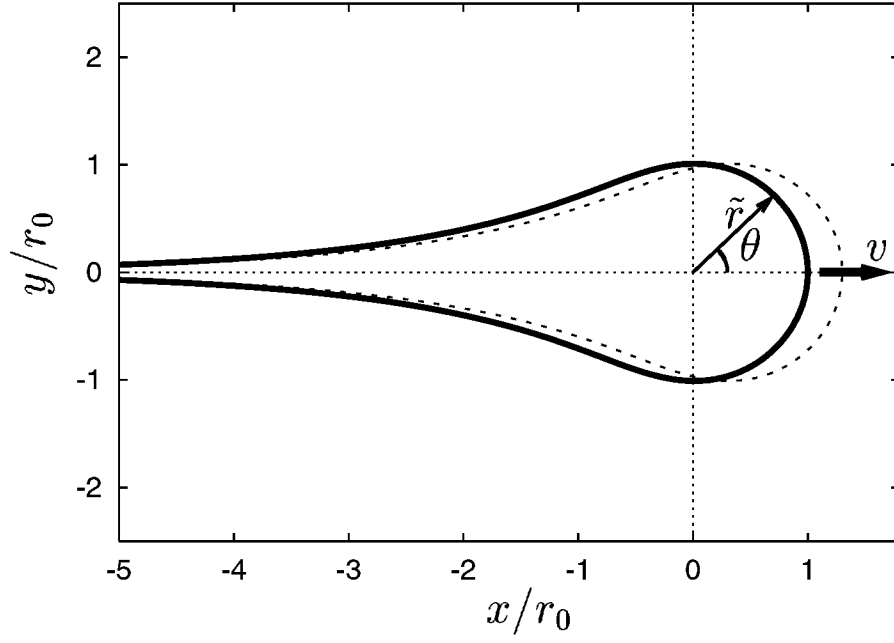


Figure 6.9: Calculated shape of the crack (without elastic displacements) driven by surface diffusion for $\Delta = 2$. The advance of the crack in positive x direction is indicated by the dashed curve. This requires the redistribution of matter along the crack by a transport mechanism.

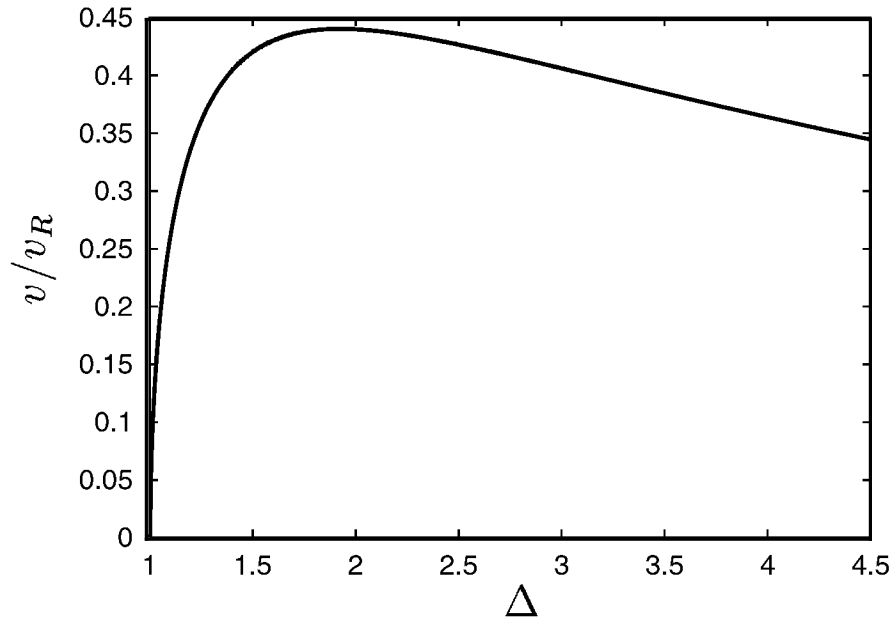


Figure 6.10: Steady state velocity of the crack versus dimensionless driving force Δ .

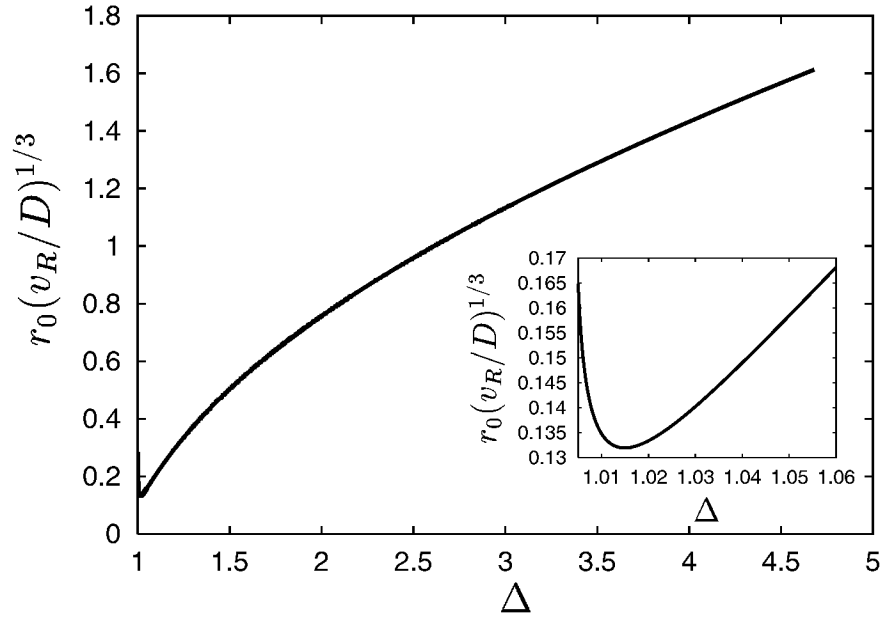


Figure 6.11: Crack tip radius r_0 versus dimensionless driving force Δ .

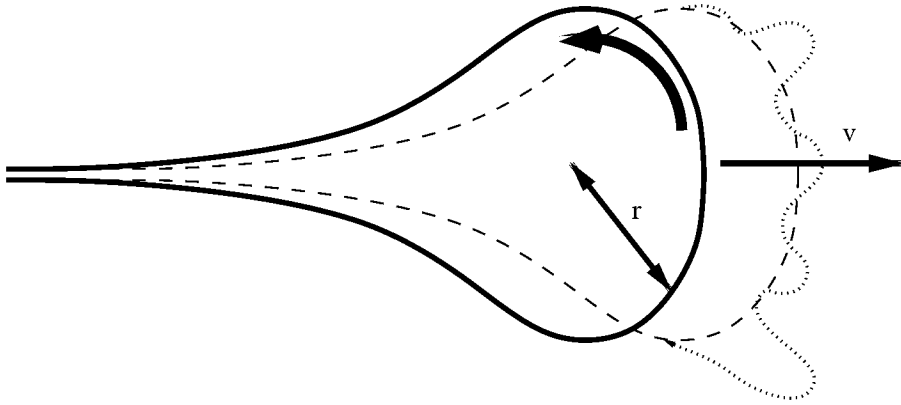


Figure 6.12: A crack which propagates by surface diffusion can become unstable due to the Grinfeld instability, as indicated by the dotted shape.

contributions which we neglected in our model, but which are obviously present in the real problem. This can be proved by simple dimensional analysis arguments: The characteristic wavelength of the ATG instability is $\lambda \sim E\alpha/\sigma_{\tau\tau}^2$ [4, 35]; in the tip region it reads $\lambda^{(tip)} \sim r_0/\Delta$. Thus, as soon as a certain critical driving force Δ_c is exceeded, the characteristic wavelength of instability fits into the tip region. The material independent number Δ_c is the threshold for the instability of the steady state solution, whereas $\Delta = 1$ is the Griffith point. Since, according to the steady state solution, v/v_R is a universal function of the dimensionless parameter Δ , the threshold of instability in terms of v/v_R is also essentially material independent. It is important to note that our steady state predictions are valid only below the threshold of instability. Thus, the main part or all of the decrease of velocity versus Δ is screened by the instability. Beyond the instability point, the behavior of the system is governed by the full time dependent evolution. Hence we expect the ATG instability to be the relevant mechanism for the experimentally observed microbranching instability [65, 26]. In contrast to the long wave instability [8, 71], this instability is localized in the tip region and cannot be suppressed by convective effects.

6.3.4 Conclusion

We have developed a self-consistent continuum model for crack propagation in homogeneous media. Both ingredients of our theory, the *linear elasticity* which is valid everywhere in the bulk and *surface diffusion* which provides a mass transport and dissipative mechanism for crack propagation, are well established. The model is essentially parameter free, leading to the prediction that two dimensionless quantities, the crack velocity v/v_R and crack tip radius $r_0(v_R/D)^{1/3}$ are universal functions of the dimensionless driving force Δ . Strictly speaking, these functions still depend weakly on the Poisson ratio. We note that these statements, together with the prediction of the tip instability above some critical velocity, are based on the general structure of our theory and do not involve the specific modeling of the surface stresses. The specific results given in the figures should differ from exact solutions only quantitatively.

It is important to realize that our model does not contradict classical theories [27], but contains more information. This allows to calculate both the crack velocity and the fracture energy, while the classical theories predict only a relation between these quantities (the integral energy balance). In our model, this energy balance is not fulfilled by approaching the Rayleigh speed limit with increasing driving force, as the classical theories predict, but by an increase of the fracture energy by tip blunting, which eventually leads to the tip instability.

At a first glance, fast crack propagation by surface diffusion seems to be counterintuitive, since the diffusion process is usually believed to be slow. However, according to our theory, the scale of velocity is set by v_R and is independent on the diffusion coefficient. The length scale of the tip is set by $(D/v_R)^{1/3}$. As we already noted, strong dissipation brings the local crack tip temperature close to the melting temperature [28, 26]. The heat is convectively transported from the hottest spot in the tip region towards the tail. Therefore, the diffusion coefficient D_s is about $10^{-7} \text{ m}^2\text{s}^{-1}$ [56] at the tip and independent of the outside temperature. With $\alpha \sim 1 \text{ Jm}^{-2}$, the interatomic distance $a \sim 10^{-10} \text{ m}$ and $v_R \sim 10^3 \text{ ms}^{-1}$, we conclude that the lengthscale of the tip is of order of atomic units. On this scale, our continuum description can be of course only qualitative.

Even more important is the fact that the term ‘surface diffusion’ should not be taken too literally. Usually, many complicated physical processes like a plastic bulk flow take place in

a small zone around the tip. Assuming that this zone is relatively thin, the mass transport can *effectively* be described by surface diffusion, where all the detailed information about the process zone is hidden in the effective surface diffusion coefficient. It can be much larger than the bare surface diffusion coefficient. This is very similar to the dynamics of the surface of a thin liquid film, where the Navier-Stokes equation in the lubrication approximation reduces to a diffusion equation for the interface profile; the effective diffusion coefficient increases cubically with the thickness of the film [63]. The relevance of atomic redistribution close to the crack surface is also confirmed by molecular dynamics simulations [83, 76].

We admit that the direct application of our model to real brittle materials might be problematic and remains an open issue. The main goal of this chapter is to introduce a well-defined theoretical model which contains explicitly mass transport and a dissipation mechanism in the process zone of the moving crack. Such a formulation, based on the mechanism of surface diffusion, is presented here; the full set of nonlocal equations leading to a free boundary problem, is given by Eqs. (6.7) and (7.18)-(7.20). Here, we have explored our main ideas by introducing a local model of stresses and solved this simplified scenario. We believe that the used scaling and counting arguments for this reduced description are the same as for the full problem.

6.3.5 “Elastic” versus “hydrodynamic” description

One of the central ingredients of our model is the linear theory of elasticity. Usually, it is assumed that all displacements are small, and therefore one does not have to discriminate between the undeformed and the deformed body. However, this is not true for a torn solid; here we discuss the implications of this effect.

In the *linear* theory of elasticity, the body is characterized by the so called *referential description*. This means that the position of individual atoms are traced while an external force is applied. The current position of an atom therefore becomes a function of the position of the same atom in the undeformed reference state (see Fig. 6.13). All quantities are

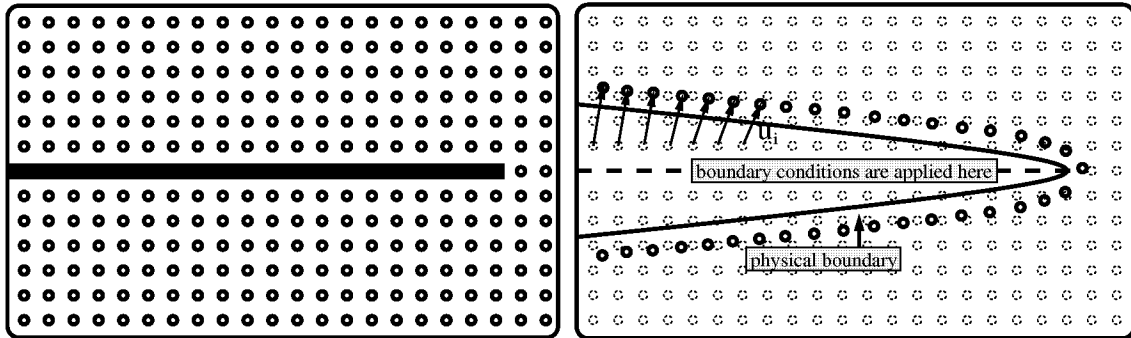


Figure 6.13: In the referential description of conventional linear elasticity, the displacement u_i of each atom is traced as a function of its original position in the undeformed state (left). If an external force is applied, all atoms are shifted, as indicated for one layer of atoms (right). The boundary conditions are not applied at the new surface but at its original location (the dashed line).

functions of the original positions. The displacement is the fundamental field from which

all other properties can be derived. In the same spirit, the crack shapes in this chapter always depict the surface contours of the undeformed body. Usually, it is assumed, that all displacements are small, and therefore it is not necessary to distinguish between the reference and displaced state. In particular, boundary conditions to the elastic problem are always applied at the undeformed interface positions.

For large deformations, this procedure can cause severe mistakes; the parabolic opening of a crack behaves like $u \sim Kr^{1/2}/E$ at a distance r from the tip and can be large; e.g. for a mathematical cut the boundary conditions are applied at the straight crack line, even though this is far away from the real boundary (see Fig. 6.13).

This effect becomes even more noticeable if an irreversible plastic flow can occur in the system [48, 22]. Then it is more reasonable to use a *spatial description* like in hydrodynamics. We give up to trace the motion of individual atoms and look for the mass density distribution $\rho(\vec{x}, t)$ at the *current* position $\vec{x}$ (see Fig. 6.14). Now the local velocity $v_i(\vec{x}, t)$ is the basic

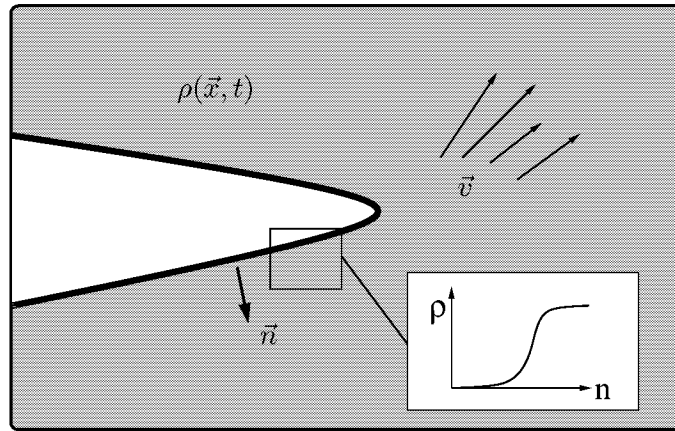


Figure 6.14: In the “hydrodynamic” description, motion is characterized by the velocity field $\vec{v}$ at fixed positions in the laboratory frame of reference, independent on the original state of the solid and not attached to atoms. The interface position can only be traced by integration of the velocity. In a phase field model, it is characterized by a strong increase of the material density ρ as function of the spatial position.

field; since we cannot follow the motion of individual atoms, displacements are not directly accessible. The interface is defined by the (spatially) sharp drop of the density and is not at a fixed position. Boundary conditions are applied at the real interface.

However, this description is much more complicated. Instead of the linear equations of elasticity for displacements, we obtain now nonlinear equations for velocities. They look very similar [49],

$$\rho \frac{dv_i}{dt} = \frac{\partial \sigma_{ij}}{\partial x_j} \quad (6.27)$$

but here the material derivative

$$\frac{d}{dt} = \frac{\partial}{\partial t} + v_k \frac{\partial}{\partial x_k} \quad (6.28)$$

appears.

At a first glance it seems that this distinction is important for the crack problem: In the tip region strains can become very large, around 10^{-1} . As we already mentioned, the

applicability of Hooke's law is very questionable for real materials here, but this is only a technical point. We claim that also the geometrical effects which we mentioned above are not too relevant.

In the tip region, the displacements are $u_i \sim u_{ij}r_0$ which is still smaller than the tip radius, and therefore the shift of the real interface is not very crucial for the application of boundary conditions. Also, we have to remember that the surface diffusion happens along the actual surface, but since it does not shift very much at the tip, this effect is also of minor influence here.

Similarly, in the tail, the opening of the crack turns out not to be excessively relevant, though it is large. Stresses decay there like $\sigma \sim K/r^{1/2}$, and since normal stresses disappear on the surface, we have

$$\sigma_{nn} \sim (\theta - \pi)K/r^{1/2} \quad (6.29)$$

for angles θ close to π . Here we assume explicitly that the undeformed shape closes far away from the tip (at $\theta = \pi$). The crack opening $u_z \sim Kr^{1/2}/E$ leads to a change of θ from almost π to $\theta^{(1)}$ with $\theta^{(1)} - \pi \sim u_z/r \sim K/(Er^{1/2})$. We can think about this as a "first order correction" to the ordinary linear description. Therefore on the deformed surface the normal stress is not zero but of order $\sigma_{nn}^{(1)} \sim K^2/(Er)$. This is a very small correction in comparison to the characteristic values $\sigma \sim K/r^{1/2}$. Hence the elastic fields are not expected to change crucially if the boundary conditions are applied on the real interface.

Since the diffusion plays its major role in the tip region, we do not expect that the deformation of the path from an almost straight line to a parabola changes a lot.

The nonlinear convective term in du_i/dt is also small: Consider the different contributions to the material derivative du/dt in the tip region. The displacement behaves like $u_i \sim Kr^{1/2}/E$, and the characteristic velocities $\partial u_i/\partial t \sim Kv/Er^{1/2}$ with the steady state velocity $v \sim (E/\rho)^{1/2}$. Since the strains are small, the convective term $v_k \partial u/\partial x_k \sim (\partial u_k/\partial t)(\partial u_i/\partial x_k) \sim K^2 v/E^2 r$ is smaller than the partial time derivative and can be neglected: Close to the Griffith point, $\Delta = 1$, the ratio $(v \partial u/\partial x)/(\partial u/\partial t) \sim \alpha^{1/2} E^{-1/2} r^{-1/2}$, which is usually much smaller or at least smaller than unity if we use typical values, $r \sim 10^{-9}$ m, $E \sim 10^{11}$ Nm $^{-2}$ and $\alpha \sim 1$ Jm $^{-2}$.

Therefore it is legitimate to use the referential description.

6.4 Summary

In this chapter we have shown that fast crack growth by surface diffusion is possible. We explained by counting arguments that the cusp singularity of the Grinfeld instability is a consequence of the static theory of elasticity which is usually used in this context. Replacing it by the dynamic theory of elasticity provides a selection mechanism for the tip radius of the deep notches which form in the late stage of the instability. Conversely, these grooves can be understood as cracks growing by surface diffusion.

In order to predict tip radius and propagation velocity as functions of the applied driving force, we developed a local stress model. It simplifies the complicated nonlinear multiscale elastodynamic free boundary problem with nonlocal effects for the steady state growth of a crack to a third order differential equation. This allows to calculate the crack shape, tip radius and crack speed. It turns out that the scale of velocity is the Rayleigh speed and crack propagation is indeed fast, though this seems to contradict the common idea of surface

diffusion at a first glance. The explanation is that the characteristic transport length, the tip radius, is of atomic scale.

We also derived that the crack tip is subject to a secondary Grinfeld instability above a certain value of the driving force, which can lead to a tip splitting.

One of the main deficits of the current description is that we do not solve the elastic problem exactly but model the stresses. In the next chapter we develop techniques to solve the full problem. This includes modifications of the chemical potential (the driving force) and also of the boundary conditions on the crack surface in order to account for kinetic effects.

Chapter 7

Solving the full problem of crack propagation by surface diffusion...

In the previous chapter we derived that fast crack growth by surface diffusion is indeed possible. We defined a set of equations which describe the steady state growth of a crack, but refrained from solving this arising complicated full problem, since it contains many difficulties:

- It is a free boundary problem, which means that the crack shape is not known in advance and has to be found self-consistently.
- The complete elastodynamic problem has to be solved. This involves multiple length scales.
- Elasticity causes complicated nonlocal effects. The chemical potential at one surface point depends on the entire shape.
- The surface diffusion process leads to the appearance of fourth order spatial derivatives in the equation of motion. As we will see later, this causes numerical difficulties.
- Boundary conditions have to be applied at different end points of the crack shape. Even for the pure local model, where a differential equation had to be solved, a shooting procedure was necessary instead of a simple initial value integration routine [58].

Therefore we invented a local stress model for a simplification of the problem and to emphasize the essential features.

In order to solve the *full* problem, several improvements have to be made. They are:

- Consistent use of the elastodynamic theory. This affects the boundary conditions and also the expression of the chemical potential. These corrections will be derived in section 7.1.
- Solution of the elastodynamic problem in the steady state regime for arbitrary crack shapes. We turn our attention to this challenge in section 7.2.
- A suitable method to find the steady state configurations of crack growth. Since the whole problem is now nonlocal, it is not described by a differential equation. A suitable method to solve this problem is given in section 7.3.

These are the necessary tools to handle the full problem; all of them are numerically implemented and tested. However, it turns out that it is hard to obtain numerical convergence, and thus we do not tackle the complicated problem of crack growth by surface diffusion here. Instead, we apply it to the related problem of the growth of a melt finger in section 7.4. Computations are very time-consuming and the results still preliminary; it will require some extended work in the future, before the surface diffusion crack problem can be solved.

7.1 The full Lagrangian

In this section we examine how the dynamical effects enter into the correct expressions for the chemical potential, which is the driving force for the surface diffusion process, and also their influence on boundary conditions. Similarly to chapter 3, we derive everything from a variational principle. The results which we obtain here are not only applicable to the crack problem but to all elastodynamic situations.

In order to describe the surface diffusion process in the quasistatic limit, we use the chemical potential as driving force. It consists of the surface energy density (per length element of the surface) and the elastic energy density (per unit volume). According to the boundary conditions, $\sigma_{nn} = \sigma_{n\tau} = 0$, it is given by the expression (2.72).

Both, the boundary conditions and the chemical potential change if inertial effects are taken into account. Here we derive the consistent expressions by deriving all necessary equations from a Lagrangian.

7.1.1 Derivation of the elastodynamic equations

We demonstrate how the equations of elastodynamics and their boundary conditions can be derived from a variational principle.

We start from the definition of the action variable:

$$S = \int_{t_0}^{t_1} dt \int_{V(t)} (T - U) dV \quad (7.1)$$

with arbitrary times t_0, t_1 and kinetic and elastic energy densities

$$T = \frac{1}{2} \rho \dot{u}_i \dot{u}_i, \quad (7.2)$$

$$U = \frac{1}{2} \sigma_{ij} u_{ij}. \quad (7.3)$$

The domain of integration is the solid body¹. Notice that this volume can be time-dependent; for our description of the crack propagation process this happens due to surface diffusion. As usual in the Lagrangian formulation, we vary both u_i and $\dot{u}_i$. This gives

$$\begin{aligned} \delta S &= \int_{t_0}^{t_1} dt \int_{V(t)} (\rho \dot{u}_i \delta \dot{u}_i - \sigma_{ij} \delta u_{ij}) dV \\ &= \int_{t_0}^{t_1} dt \left\{ \int_{V(t)} \left(\rho \dot{u}_i \delta \dot{u}_i + \frac{\partial \sigma_{ij}}{\partial x_j} \delta u_i \right) dV - \int_{\partial V(t)} \sigma_{ni} \delta u_i dS \right\}. \end{aligned} \quad (7.4)$$

¹In the referential description of the linear theory of elasticity, this is the *undeformed* body.

Now we examine the first term

$$\delta A = \int_{t_0}^{t_1} dt \int_{V(t)} \rho \dot{u}_i \delta \dot{u}_i dV \quad (7.5)$$

in more detail. We start from the expression

$$\frac{d}{dt} \int_{V(t)} \rho \dot{u}_i \delta u_i dV = \int_{V(t)} (\rho \ddot{u}_i \delta u_i + \rho \dot{u}_i \delta \dot{u}_i) dV + \int_{\partial V(t)} v_n \rho \dot{u}_i \delta u_i dS. \quad (7.6)$$

v_n is the normal velocity of the interface. It is positive if the solid extends. Therefore we obtain

$$\delta A = \int_{t_0}^{t_1} dt \left\{ \frac{d}{dt} \int_{V(t)} \rho \dot{u}_i \delta u_i dV - \int_{V(t)} \rho \ddot{u}_i \delta u_i dV - \int_{\partial V(t)} v_n \rho \dot{u}_i \delta u_i dS \right\}. \quad (7.7)$$

The first bulk integral does not contribute since we have to demand that all variations disappear at t_0 and t_1 [32]. Consequently, we obtain the full variation of the action variable

$$\delta S = \int_{t_0}^{t_1} dt \left\{ \int_{V(t)} [-\rho \ddot{u}_i \delta u_i + \frac{\partial \sigma_{ij}}{\partial x_j} \delta u_i] dV - \int_{\partial V(t)} [\sigma_{ni} \delta u_i + v_n \rho \dot{u}_i \delta u_i] dS \right\}. \quad (7.8)$$

From the condition that the action must be stationary for all kind of variations, we finally obtain the elastodynamic equations and also the boundary conditions:

$$\frac{\partial \sigma_{ij}}{\partial x_j} = \rho \ddot{u}_i, \quad (7.9)$$

$$\sigma_{ni} = -v_n \rho \dot{u}_i. \quad (7.10)$$

Equation (7.9) is precisely Newton's equation of motion; Eq. (7.10) reflects the momentum conservation at a moving interface [27].

7.1.2 Derivation of the chemical potential

Here we show how the kinetic energy appears in the chemical potential. We justify why not the *energy* density but the density of the *Lagrangian* enters into this expression.

The question arises how kinetic effects enter into the chemical potential μ_{el} . A natural guess to generalize the static result that μ_{el} is the elastic energy density would be $\mu_{el} = \Omega(U + T)$, with Ω being the atomic volume. However, it turns out that this is not correct. Instead, one has to derive it from the Lagrangian, and therefore one finally obtains

$$\mu_{el} = \Omega(U - T). \quad (7.11)$$

We claim that the chemical potential is given by the variation of the Lagrangian

$$L = \int_{V(t)} (T - U) dV = \int_{V(t)} \left(\frac{1}{2} \rho \dot{u}_i \dot{u}_i - \frac{1}{2} \sigma_{ij} u_{ij} \right) dV \quad (7.12)$$

with respect to the interface position at a fixed time:

$$\mu = -\Omega \frac{\delta L}{\delta n}. \quad (7.13)$$

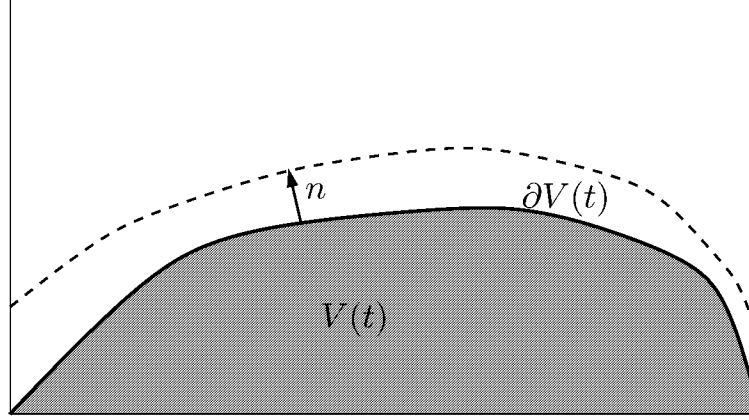


Figure 7.1: How does the energy of the system change if the solid extends in a direction normal to its interface?

This immediately leads to the result (7.11). The reason for this relation becomes clear by computation of the energy dissipation rate. The energy of the system is

$$E = \int_{V(t)} (T + U) dV = \int_{V(t)} \left(\frac{1}{2} \rho \dot{u}_i \dot{u}_i + \frac{1}{2} \sigma_{ij} u_{ij} \right) dV. \quad (7.14)$$

The energy changes in time due to the influence of external forces at the boundary and dissipation due to motion of the interface. For the moment, the origin of this motion is not relevant, and therefore we do not specify it here. Surface diffusion is a possible example.

Then the total dissipation rate is given by

$$\begin{aligned} \frac{dE}{dt} &= \int_{\partial V(t)} v_n (T + U) dS + \int_{V(t)} (\rho \dot{u}_i \ddot{u}_i + \sigma_{ij} \dot{u}_{ij}) dV \\ &= \int_{\partial V(t)} v_n (T + U) dS + \int_{\partial V(t)} \sigma_{ni} \dot{u}_i dS \\ &= \int_{\partial V(t)} v_n (T + U) dS - \int_{\partial V(t)} v_n \rho \dot{u}_i \dot{u}_i dS \\ &= \int_{\partial V(t)} v_n (U - T) dS. \end{aligned} \quad (7.15)$$

The second step follows from integration by parts of the last term and application of the bulk equilibrium condition (7.9). The following step uses the boundary condition (7.10).

Comparison with the definition of the chemical potential,

$$\frac{dE}{dt} = \frac{1}{\Omega} \int v_n \mu ds, \quad (7.16)$$

leads to the result (7.11). It shows that indeed the difference $T - U$ instead of the energy density $T + U$ is responsible for interface motion. Hence the correct expression for the chemical potential, including surface energy, is

$$\mu = \Omega \left(\frac{1}{2} \sigma_{ik} u_{ik} - \frac{1}{2} \rho \dot{u}_i^2 - \alpha \kappa \right). \quad (7.17)$$

7.1.3 The dynamical formulation of crack propagation

Application of the preceding results to the crack propagation process by surface diffusion modifies the equation which we used in the previous chapter. Now we start to solve the complete problem, and therefore we also push up all exact equations.

The bulk equations of elasticity,

$$\frac{\partial \sigma_{ij}}{\partial x_j} = \rho \ddot{u}_i, \quad (7.18)$$

are subject to the boundary conditions on the crack surface (surface of discontinuity) [27]

$$\sigma_{in} + \rho \dot{u}_i v_n = 0, \quad (7.19)$$

with the mass density ρ and the elastic displacement field u_i . This is just the momentum balance equation on the free surface which moves with normal velocity v_n . Notice that this velocity is not the displacement rate $\dot{u}_n$ but results from motion of the interface due to surface diffusion. Finally, the expression for the chemical potential on the crack surface should also be corrected compared to the static case:

$$\mu = \Omega \left(\frac{1}{2} \sigma_{ik} u_{ik} - \frac{1}{2} \rho \dot{u}_i^2 - \alpha \kappa \right). \quad (7.20)$$

Eqs. (7.18)-(7.20), together with surface diffusion, Eq. (6.7), and given loading configuration describe the crack propagation in our model. We note that inertial effects appear not only in the bulk equations of elasticity but also in the boundary conditions and in the expression for the chemical potential.

7.2 The stress field expansion

One of the main ingredients to the full solution of the crack problem is the solution of the elastic problem. Here the difficulty arises that the shape of the crack is not known in advance and changes during the propagation process. A natural approach would be to consider a finite crack with a time-dependent shape and to discretize the surrounding solid by a grid and to use time-dependent finite-element or finite-difference methods to solve the full elastic equations. This causes the problem that one has to resolve both the spatially strongly varying fields in the tip region of typical extend r_0 , but also the whole crack of length L ; both quantities are relevant for the stress field in the most important tip region: r_0 determines the stress singularity and L appears naturally in the stress intensity factor. Therefore this approach requires many grid points and extremely high computation times.

Since we are basically interested in the near-tip behavior, it is more reasonable to use analytical knowledge about the far field and the structure of the fields in the tip region. In this sense, we follow the ideas which we already used for the local model. However, now we try to solve the elastic problem exactly in the limit $L \gg r_0$. This leads to the important simplification of a separation of lengthscales.

For an ideal crack (a mathematical cut) with infinitely sharp tip, stresses behave like

$$\sigma_{ij} \sim K_I^{(dyn)} \frac{1}{r^{1/2}} \quad (7.21)$$

at distances r from the crack tip. $K_I^{(dyn)}$ is the dynamical stress intensity factor, which will be explained in section 7.2.3. A derivation for the near tip-behavior will be given in the next section.

For a blunt crack tip, the idea is to present the stress field as a series expansion

$$\sigma_{ij} \sim K_I^{(dyn)} \frac{1}{r^{1/2}} \left(1 + \frac{a_1}{r} + \frac{a_2}{r^2} + \dots \right). \quad (7.22)$$

Weight factors a_i in front of the higher modes are adjusted such that the elastic boundary conditions are fulfilled on the crack shape. Far away, the crack looks again like a mathematical cut; here all higher modes have decayed, and we observe the normal $r^{-1/2}$ behavior.

These higher modes are not chosen arbitrarily. Their radial and angular behavior is determined by the fact that they are eigenmodes of the straight mathematical cut. They fulfill the elastodynamic bulk equations.

Another simplification comes the explicit usage of the steady state situation. We immediately assume that the crack shape does not change in a co-moving frame of reference and that the propagation velocity is constant.

The analytic part is divided into two parts: First, we address the problem to find the eigenfunctions which we use for the expansion. They are derived in the next section. In section 7.2.2 we provide the tools to solve the elastodynamic steady state problem for arbitrary crack shapes. The solution is unique up to the scalar factor, the stress intensity factor. We discuss this second problem in section 7.2.3. Afterwards, in section 7.2.4, we present first results and checks for the applicability and quality of the ansatz to solve elastic problems.

7.2.1 The eigenmodes of the straight crack

In this section we derive expressions for the eigenmodes of a straight, semi-infinite crack which advances with a velocity v . Later, we will use this set of eigenfunctions as a base to solve complicated elastodynamic steady-state problems for arbitrary crack shapes.

We use a two-dimensional plane strain solid which is subjected to a mode I loading. This means that the applied tensile force acts perpendicular to the crack (see Fig. 7.2). The boundary conditions, here $\sigma_{nn} = \sigma_{n\tau} = 0$, on the crack have to be fulfilled. Also, far away from the crack, the stress field must reach its homogeneous value. We do not consider it here and concentrate on the behavior near the crack tip. If we talk about the stress field, we always mean the *singular* part of the field and suppress the constant contribution.

We start with a description in the laboratory frame of reference and assume that the crack moves with a constant velocity v . The elastic displacements u_i have to fulfill Newton's equation of motion

$$\frac{\partial \sigma_{ij}}{\partial x_j} = \rho \ddot{u}_i. \quad (7.23)$$

We introduce two real functions $\phi(x, y, t)$ and $\psi(x, y, t)$ and define displacements u_i through [59]

$$u_x = \frac{\partial \phi}{\partial x} + \frac{\partial \psi}{\partial y}, \quad u_y = \frac{\partial \phi}{\partial y} - \frac{\partial \psi}{\partial x}. \quad (7.24)$$

Then (7.23) obviously becomes a third order equation; one can easily check that it can be integrated once. Therefore we obtain two decoupled, second order equilibrium equations:

$$c_d^2 \nabla^2 \phi = \frac{\partial^2 \phi}{\partial t^2}, \quad c_s^2 \nabla^2 \psi = \frac{\partial^2 \psi}{\partial t^2}. \quad (7.25)$$

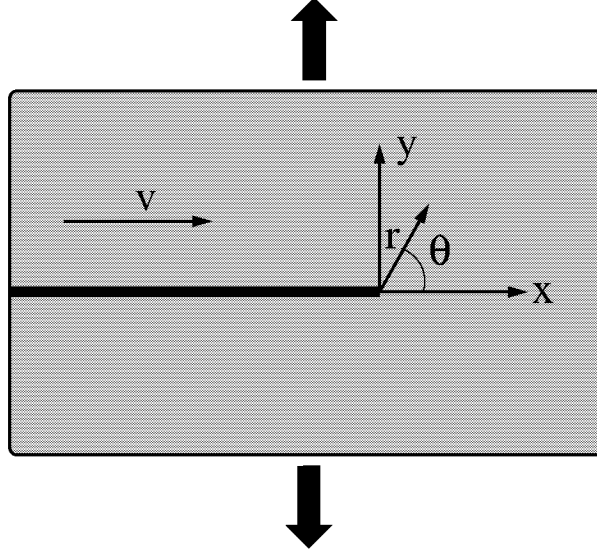


Figure 7.2: The straight mathematical and semi-infinite cut which advances in positive x direction with velocity v .

They contain the shear and dilatational velocities (2.50) and (2.51). We perform a transformation into a co-moving frame of reference ($v < c_s < c_d$) and rescale the axes,

$$x \rightarrow x - vt, \quad (7.26)$$

$$y_d = \alpha_d y, \quad (7.27)$$

$$y_s = \alpha_s y, \quad (7.28)$$

with

$$\alpha_d^2 = 1 - (v/c_d)^2, \quad \alpha_s^2 = 1 - (v/c_s)^2. \quad (7.29)$$

From now on we describe everything in the frame of reference where the crack is at rest. We write formally

$$\phi_0(x, y_d, t) = \phi(x, y, t), \quad \psi_0(x, y_s, t) = \psi(x, y, t). \quad (7.30)$$

In the steady state situation, where all time derivatives disappear in the co-moving frame of reference, the two inhomogeneous equations become just normal (homogeneous) Laplace equations, which are relatively easy to solve,

$$\frac{\partial^2 \phi_0}{\partial x^2} + \frac{\partial^2 \phi_0}{\partial y_d^2} = 0, \quad \frac{\partial^2 \psi_0}{\partial x^2} + \frac{\partial^2 \psi_0}{\partial y_s^2} = 0. \quad (7.31)$$

We also introduce polar coordinates with origin at the sharp tip of the crack,

$$r_d e^{i\theta_d} = x + iy_d, \quad r_s e^{i\theta_s} = x + iy_s. \quad (7.32)$$

Similar to section 2.5, we are interested in semi-infinite cracks which are aligned along the negative real axis. Therefore we make the ansatz

$$\phi_0 = A_n r_d^n \cos n\theta_d, \quad (7.33)$$

$$\psi_0 = -B_n r_s^n \sin n\theta_s. \quad (7.34)$$

It is adjusted to a mode I loading and a symmetry with respect to the x axis. Similarly to the static crack, all integer and half integer values of n ,

$$n = \pm 1/2, \pm 3/2, \pm 5/2, \dots, 0, \pm 1, \pm 2, \dots \quad (7.35)$$

lead to solutions, since they fulfill the boundary conditions $\sigma_{nn} = \sigma_{\tau\tau} = 0$ (compare chapter 2.5). But again, $n \geq 2$ leads to non-decaying fields for $r \rightarrow \infty$ which contradict the homogeneous far-field, and $n < 3/2$ leads to a divergent energy density $dU_{el} \sim r\sigma^2 dr/E$ near the infinitely sharp tip of the mathematical cut, $r \rightarrow 0$. Therefore only $n = 3/2$ remains here. For this mode, we obtain also from boundary conditions

$$B_{3/2} = \frac{2\alpha_d}{1 + \alpha_s^2} A_{3/2}. \quad (7.36)$$

The dimension of $A_{3/2}$ is $[A_{3/2}] = (length)^{1/2}$. It gives a scalar degree of freedom which is nothing else than the stress intensity factor: $K \sim EA_{3/2}$. Notice that we describe a semi-infinite crack, $L = \infty$, but the stress intensity factor $K \sim PL^{1/2}$ requires the existence of a macroscopic lengthscale L in the system which is naturally not present here. Thus this degree of freedom remains.

The stress fields corresponding to the main mode $n = 3/2$ are

$$\sigma_{11} = \frac{3}{4}\mu A_{3/2} \left[(1 + 2\alpha_d^2 - \alpha_s^2) \frac{\cos \theta_d/2}{r_d^{1/2}} - \frac{4\alpha_s\alpha_d \cos \theta_s/2}{1 + \alpha_s^2} \frac{1}{r_s^{1/2}} \right], \quad (7.37)$$

$$\sigma_{12} = \frac{3}{2}\mu A_{3/2} \alpha_d \left[\frac{\sin \theta_d/2}{r_d^{1/2}} - \frac{\cos \theta_s/2}{r_s^{1/2}} \right], \quad (7.38)$$

$$\sigma_{22} = \frac{3}{4}\mu A_{3/2} \left[-(1 + \alpha_s^2) \frac{\cos \theta_d/2}{r_d^{1/2}} + \frac{4\alpha_s\alpha_d \cos \theta_s/2}{1 + \alpha_s^2} \frac{1}{r_s^{1/2}} \right]. \quad (7.39)$$

These dynamic singular fields also contain the limiting case $v \rightarrow 0$ of the static crack and reproduce the fields (2.37)².

The amplitude $A_{3/2}$ is related to the dynamic stress intensity factor [27]

$$A_{3/2} = \frac{8(1 + \nu)(1 + \alpha_s^2)}{3E(2\pi)^{1/2}(4\alpha_s\alpha_d - (1 + \alpha_s^2))} K_I^{(dyn)}. \quad (7.40)$$

Notice that this expression becomes singular for $v \rightarrow 0$.

The other non-integer modes turn out to be relevant for crack shapes with a finite tip radius.

Displacements and strains can also be calculated. For general n , A_n and B_n , they are

$$u_x = A_n r_d^{n-1} n \cos[(n-1)\theta_d] - B_n \alpha_s r_s^{n-1} n \cos[(n-1)\theta_s], \quad (7.41)$$

$$u_y = -A_n r_d^{n-1} n \alpha_d \sin[(n-1)\theta_d] + B_n r_s^{n-1} n \sin[(n-1)\theta_s]. \quad (7.42)$$

²Notice that the static fields contain not only terms $\sin(\theta/2)$ and $\cos(\theta/2)$ but also terms $\sin(3\theta/2)$ and $\cos(3\theta/2)$ which are not present in (7.37)-(7.39). This seems to contradict the derivability of the static fields from the dynamic ones. However, the dynamic fields are singular for $v = 0$, and only the limit $v \rightarrow 0$ can be evaluated; then one reproduces indeed the static fields; corrections are of order $(v/c_s)^2$. Alternatively, one can use the case $v = 0$ from the very beginning. Then it turns out that the ansatz (7.33) and (7.34) does not produce two independent solutions with weight factors A_n and B_n . Another independent mode can be constructed using $n - 2$ instead in the angular dependence, in agreement with the static calculations in section 2.5.

Strains can be derived from

$$\begin{aligned} u_{xx} &= u_{x,x} = \frac{\partial u_x}{\partial x} \\ &= A_n r_d^{n-2} n(n-1) \cos[(n-2)\theta_d] - B_n \alpha_s r_s^{n-2} n(n-1) \cos[(n-2)\theta_s], \end{aligned} \quad (7.43)$$

$$\begin{aligned} u_{yy} &= u_{y,y} = \frac{\partial u_y}{\partial y} \\ &= -A_n \alpha_d^2 r_d^{n-2} n(n-1) \cos[(n-2)\theta_d] + B_n \alpha_s r_s^{n-2} n(n-1) \cos[(n-2)\theta_s], \end{aligned} \quad (7.44)$$

$$u_{x,y} = -A_n \alpha_d r_d^{n-2} n(n-1) \sin[(n-2)\theta_d] + B_n \alpha_s^2 r_s^{n-2} n(n-1) \sin[(n-2)\theta_s], \quad (7.45)$$

$$u_{y,x} = -A_n \alpha_d r_d^{n-2} n(n-1) \sin[(n-2)\theta_d] + B_n r_s^{n-2} n(n-1) \sin[(n-2)\theta_s] \quad (7.46)$$

$$u_{xy} = \frac{1}{2}(u_{x,y} + u_{y,x}). \quad (7.47)$$

Stresses can be calculated using Hooke's law.

In summary, we derived the singular part of the elastic fields for a semi-infinite mathematical cut which is propagating with a constant velocity v . For this specific case, only one solution with behavior $\sigma \sim r^{-1/2}$ is possible; the strength of the field is related to the dynamical stress intensity factor. All other singular modes with decay $\sigma \sim r^{-3/2}$, $\sigma \sim r^{-5/2}$, ... lead to a divergent energy density at the crack tip, but also fulfill the boundary conditions. They will be required later when we discuss cracks with blunt tips. Then these modes appear as well.

7.2.2 Solution of the elastic problem

Here we present a technique to solve the elastodynamic problem of a semi-infinite crack which is not a mathematical cut.

In order to solve the elastic problem for a non-mathematical cut, we expand the stress field in the set of eigenmodes which we obtained above. Since the tip is not infinitely sharp, one cannot exclude contributions with $n < 3/2$ due to the constraint $r > r_0$. On the scale $r_0 \ll r \ll L$ the crack still looks like a straight, semi-infinite mathematical cut, and therefore exhibits the far-field behavior of Eqs. (7.37)-(7.39). This forbids values of n with $n \geq 2$.

The attempt to solve the problem is to present the total field by superposition

$$\phi_0 = A_{3/2} r_d^{3/2} \cos(3\theta_d/2) + \sum_{\{n < 3/2\}} A_n r_d^n \cos n\theta_d, \quad (7.48)$$

$$\psi_0 = -B_{3/2} r_d^{3/2} \sin(3\theta_d/2) - \sum_{\{n < 3/2\}} B_n r_d^n \sin n\theta_d. \quad (7.49)$$

Each eigenmode fulfills by construction the elastic equations, therefore the superposition does it as well. The coefficients $A_{3/2}$ and $B_{3/2}$ are fixed by Eqs. (7.40) and (7.36) for the correct far-field behavior. All other modes decay faster and do not contribute to the asymptotics. Only the half-integer modes $n = 1/2, -1/2, -3/2, \dots$ appear here. This corresponds to a series expansion of stresses

$$\sigma_{ij} \sim \frac{K}{r^{1/2}} \left(1 + \frac{\alpha_1}{r} + \frac{\alpha_2}{r^2} + \dots \right). \quad (7.50)$$

This is also asserted by the known series expansions for certain crack geometries which contain only half-integer modes, like a parabolic crack (see also section 7.2.4). No rigorous proof for

this restriction to half integer modes can be given here - currently, it is simply a guess. The only arguments are that the Laurent-like series (7.50) should already be complete and that the expansion of analytically known stress fields for specific problems does not show modes with other values of n . Notice that the coefficients A_n and B_n are related to each other only for $n = 3/2$. This is necessary to reproduce the correct far fields. The other coefficients are determined by the boundary conditions (7.10)

$$\sigma_{in} + \rho v_n \dot{u}_i = 0. \quad (7.51)$$

Normal motion of the interface originates from surface diffusion; in the steady state case of a crack propagating in positive x direction with velocity v , we have

$$v_n = v n_x, \quad (7.52)$$

with the x component of the interface normal vector n_x . Since this cannot be fulfilled at all interface points as long as we use only a finite series, we determine the coefficients by minimizing the residuum

$$Res = \int (\sigma_{in} + \rho v_n \dot{u}_i)^2 ds. \quad (7.53)$$

The main contribution to the integral comes from the tip region, which assures the best approximation of the exact solution in this region. The minimum of Res with respect to a variation of the coefficients A_n and B_n leads to a inhomogeneous set of linear equations for these coefficients. We developed a C++ program to solve this problem by QR decomposition of the characteristic matrix [58]. Since this procedure is straightforward, we refrain from explaining it.

Summing up, we developed a method to solve elastodynamic crack problems for arbitrary shapes. The coefficient for the used series expansion are determined by minimization of the stress residuum (7.53) to a best fulfillment of the boundary conditions.

7.2.3 Static and dynamic stress intensity factors

Since the angular and radial dependence of the stress field is now understood in the tip region, we address the problem of the stress intensity factor. We have to discriminate between the static and the dynamic stress intensity factor. They contain both all information about the size of the sample, crack length and structure.

The strength of the stress field in the tip region is controlled by the stress intensity factor. Also for a moving crack it is defined by the value of the stress in front of the crack, $\theta = 0$,

$$K_I^{(dyn)} = \lim_{r \rightarrow \infty} (2\pi r)^{1/2} \sigma_{zz}(r). \quad (7.54)$$

For $v = 0$ we obtain the static stress intensity factor, which behaves as

$$K_I^{(stat)} \sim PL^{1/2}, \quad (7.55)$$

with the length of the crack L and the external stress P . The static and dynamic stress intensity factor are related by a function $f(v)$ of the propagation velocity [27]

$$K_I^{(dyn)} = f(v) K_I^{(stat)}. \quad (7.56)$$

This function depends on the geometry of the sample. In this sense, not only the local properties in the vicinity of the tip become relevant for the singular field, but also some “macroscopic” properties. In particular, one tip “feels” the existence of the other one, even if they are far away from each other, as one can see from the following examples:

1. The Broberg problem [27]. A mathematical cut with tips propagating with constant velocity v in *opposite* directions. In this case, of course $K_I^{(stat)} = K_I^{(dyn)}$ for $v = 0$, but $f(v)$ decreases for increasing v and reaches zero at the Rayleigh speed, $v = v_R$.
2. The Yoffe problem [27]. Also a mathematical cut, but here the cracks move in the *same* direction, with velocity v . Therefore the crack length is constant and the whole crack travels through the solid. Of course, for mode I , this is a very artificial situation, and we get the result $K_I^{(dyn)} = K_I^{(stat)}$ for all velocities. At a first glance, this is very surprising, but we can imagine to switch to the co-moving frame of reference where the crack is at rest, and then it is clear that both stress intensity factors must coincide.
3. Crack in a narrow strip [26]. If the length of the crack is much longer than the strip width, the stress intensity factor becomes a velocity dependent constant, even if the crack elongates.

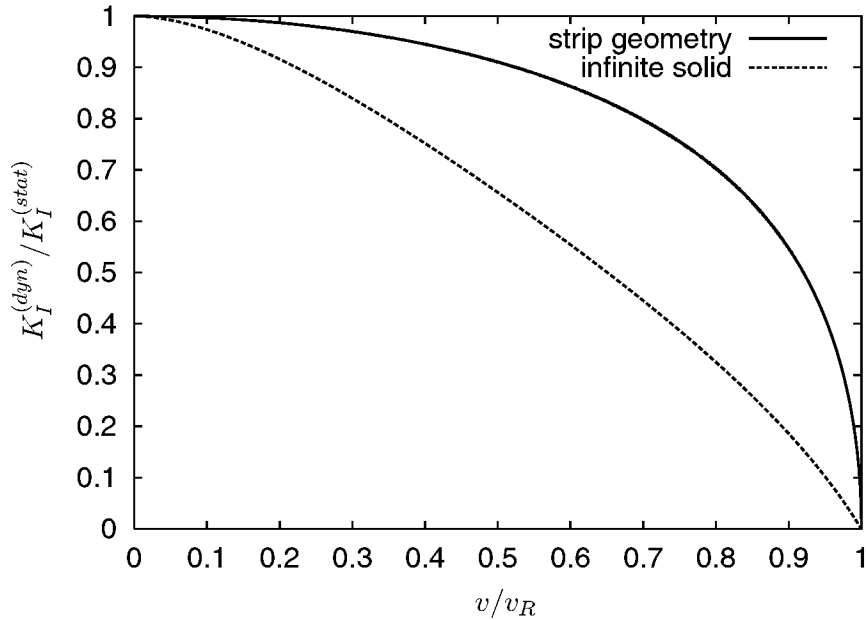


Figure 7.3: The dynamic stress intensity factor for the strip geometry and the infinite solid (Broberg problem). $\nu = 0.2$ in both cases.

For the Broberg problem, the velocity relation is given by [27]

$$\frac{K_I^{(dyn)}}{K_I^{(stat)}} = -\frac{I(b/h)R(h)}{b^2 h \sqrt{h^2 - a^2}}, \quad (7.57)$$

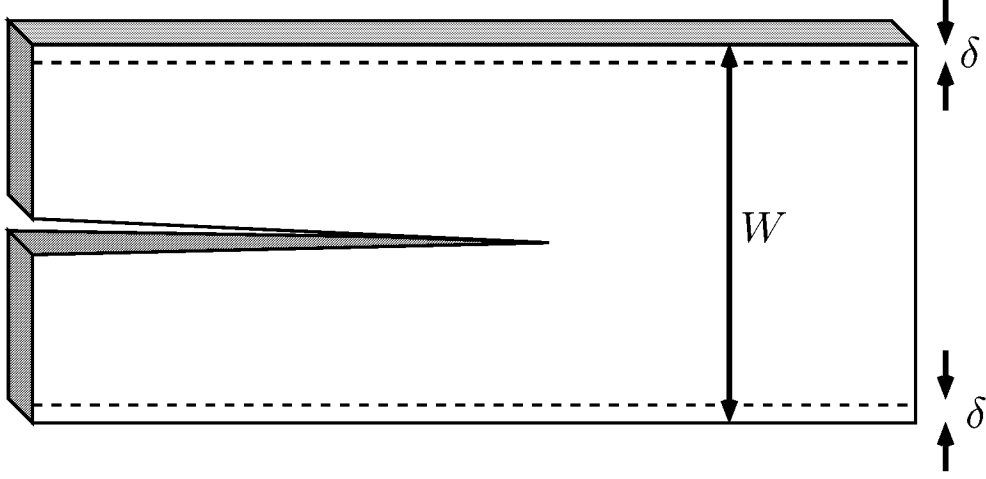


Figure 7.4: The semi-infinite crack in a strip.

where we use $h = v^{-1}$, $a = c_d^{-1}$ and $b = c_s^{-1}$, and therefore $0 < a < b$. $R(h)$ is the Rayleigh function

$$R(h) = (b^2 - 2h^2)^2 + 4h^2\sqrt{a^2 - h^2}\sqrt{b^2 - h^2}. \quad (7.58)$$

The function $I(b/h)$ can be expressed only through an integral

$$I(b/h) = \frac{b^2}{h} \left[\int_0^\infty \frac{R(i\eta)}{(h^2 + \eta^2)^{3/2} \sqrt{a^2 + \eta^2}} d\eta \right]^{-1}. \quad (7.59)$$

For $v/c_s \rightarrow 0$, it follows $I(b/h) \rightarrow 1 - \nu$.

In the strip geometry the energy dissipation rate is [26]

$$J = \frac{2Ev\delta^2}{W(1 - \nu^2)}, \quad (7.60)$$

with the strip width W and opening 2δ (see Fig. 7.4).

On the other hand, the same expression gives in general

$$J = K_I^{(dyn)2} v \frac{1 + \nu}{E} \frac{\alpha_d(1 - \alpha_s^2)}{4\alpha_d\alpha_s - (1 + \alpha_s^2)^2}, \quad (7.61)$$

which tends to

$$J = K_I^{(stat)2} v \frac{1 - \nu^2}{E}. \quad (7.62)$$

Comparison with (7.60) gives

$$K_I^{(dyn)} = K_I^{(stat)} \left((1 - \nu) \frac{4\alpha_d\alpha_s - (1 + \alpha_s^2)^2}{\alpha_d(1 - \alpha_s^2)} \right)^{1/2}. \quad (7.63)$$

We already saw in chapter 2.4 that for a fixed applied force, the propagation velocity can become only constant in a strip geometry. Otherwise, the stress intensity factor increases with

the length of the crack, and this also alters the propagation velocity similar to the results of the local model. Therefore, we use the strip geometry and the expression (7.63) for the ratio between static and dynamic stress intensity factor. The experimentally accessible quantity is $K_I^{(stat)}$, and for steady state growth this gives consistently a constant dynamic stress intensity factor.

7.2.4 Numerical results

Here we present numerical calculations which make use of the expansion technique to solve elastodynamic problems. In particular, we study the quality of solution for a parabolic crack and compare it to analytical results. Also, we define an effective driving force which can be used to measure the quality of solution.

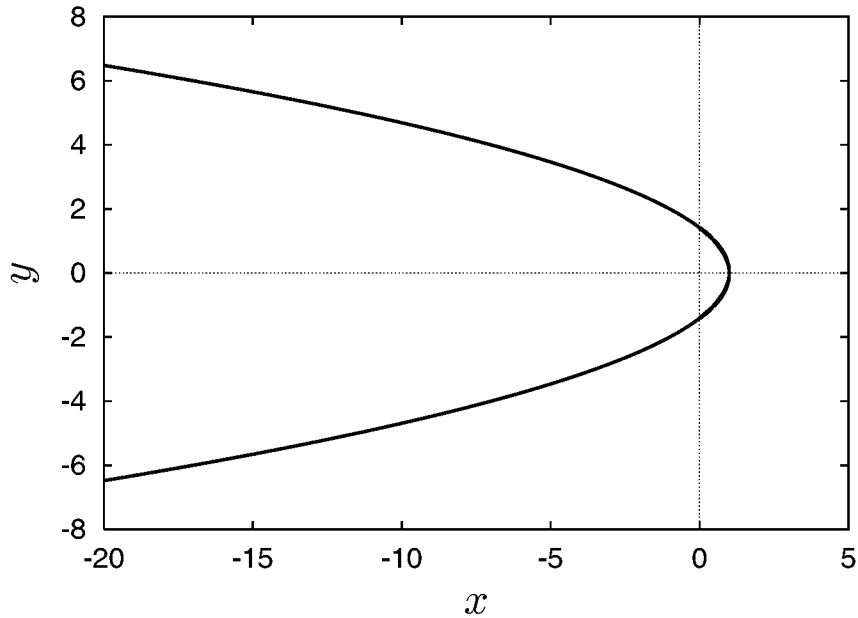


Figure 7.5: Parabolic crack shape as used for testing the elastodynamic expansion technique. The tip is located at $x = 1$ and has radius $r = 1$.

The propagation of the crack changes both the elastic and surface energy content of the system. We can balance the energy dissipation rate at the crack surface to the decrease of the far-field elastic energy. On the one hand, the elastic power can be expressed by

$$J_{el} = \frac{1}{\Omega} \int_S v_n \mu_{el} ds, \quad (7.64)$$

with the local normal velocity v_n . The integral is performed along the whole crack shape S . The elastic contribution to the chemical potential is

$$\mu_{el} = \Omega \left(\frac{1}{2} \sigma_{ij} u_{ij} - \frac{1}{2} \rho \dot{u}_i^2 \right). \quad (7.65)$$

For steady state,

$$v_n = v \cos \theta, \quad (7.66)$$

where v is the steady state velocity in x direction. The angle θ is the inclination angle of the interface normal to the x -axis. On the other hand, the dissipation rate for steady state propagation can be calculated through the far field [26]

$$J_{el} = K_I^{(stat)^2} \frac{1 - \nu^2}{E} v = 2\alpha v \Delta, \quad (7.67)$$

with the dimensionless driving force

$$\Delta = \frac{K_I^{(stat)^2} (1 - \nu^2)}{2E\alpha}. \quad (7.68)$$

The curvature contribution is similarly given by

$$\mu_s = -\Omega\alpha\kappa, \quad J_s = \frac{1}{\Omega} \int_S v_n \mu_s ds. \quad (7.69)$$

In the steady state case, it can be evaluated explicitly

$$J_s = -2\alpha v, \quad (7.70)$$

where we assumed a semi-infinite crack. This expression reflects the elongation of the total crack. The Griffith point is determined by the vanishing of $J_{tot} = J_{el} + J_s$. This gives the known value $\Delta = 1$.

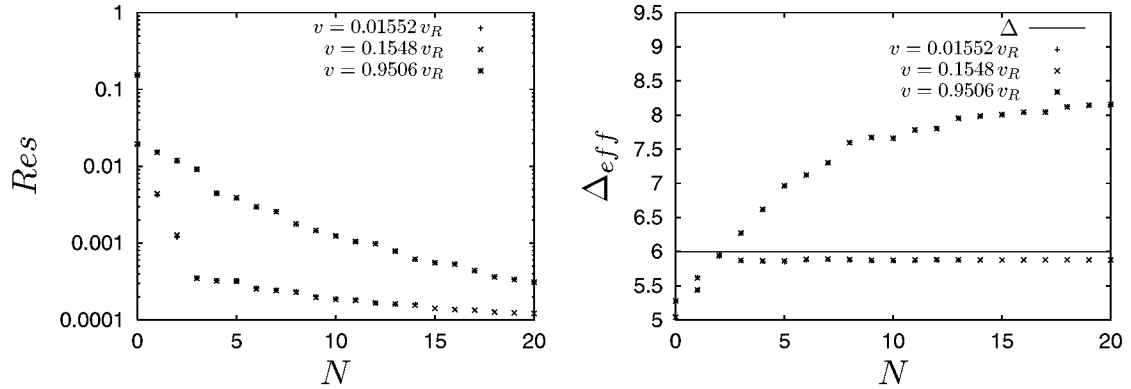


Figure 7.6: Residuuum and effective driving force for the parabolic crack (Fig. 7.5) as function of the number of expansion modes $2N + 2$. The used values are (in dimensionless units) $E = 0.08$, $\nu = 0.2$, $\rho = 1$. The driving force is $\Delta = 6$. For the two lower velocities the curves are almost indistinguishable; with higher propagation velocity the convergence becomes worse.

In our numerical approach, the elastic boundary conditions are not fulfilled exactly. Therefore the two expressions (7.64) and (7.67) differ, and their deviation is a measure for the quality of the solution of the elastic problem. We can define an effective driving force

$$\Delta_{eff} := \frac{1}{2\alpha} \int_S \cos \theta \left(\frac{1}{2} \sigma_{ij} u_{ij} - \frac{1}{2} \rho \dot{u}_i^2 \right) ds. \quad (7.71)$$

Only if the boundary conditions are fulfilled exactly, we have $\Delta = \Delta_{eff}$.

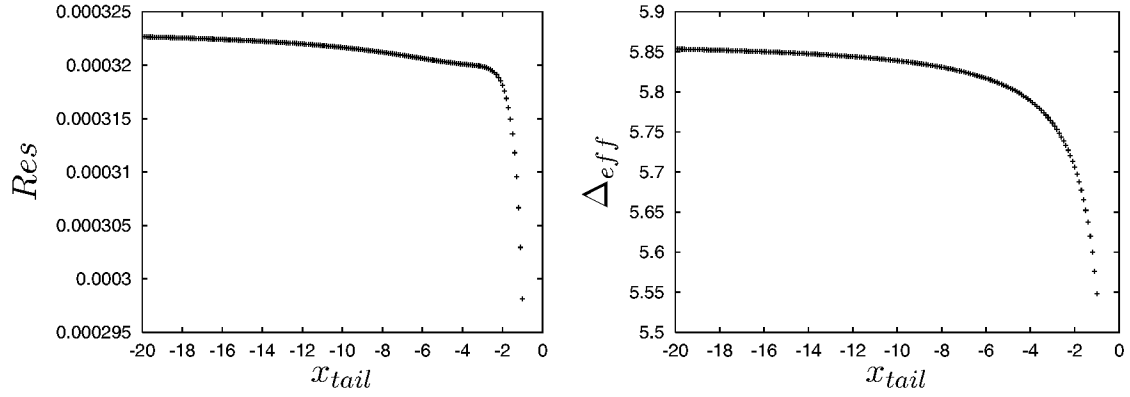


Figure 7.7: Dependence of residuum and effective driving force on the tail crop point x_{tail} for the parabolic crack in Fig. 7.5. The steady state velocity is $v = 0.01552 v_R$ and $N = 5$.

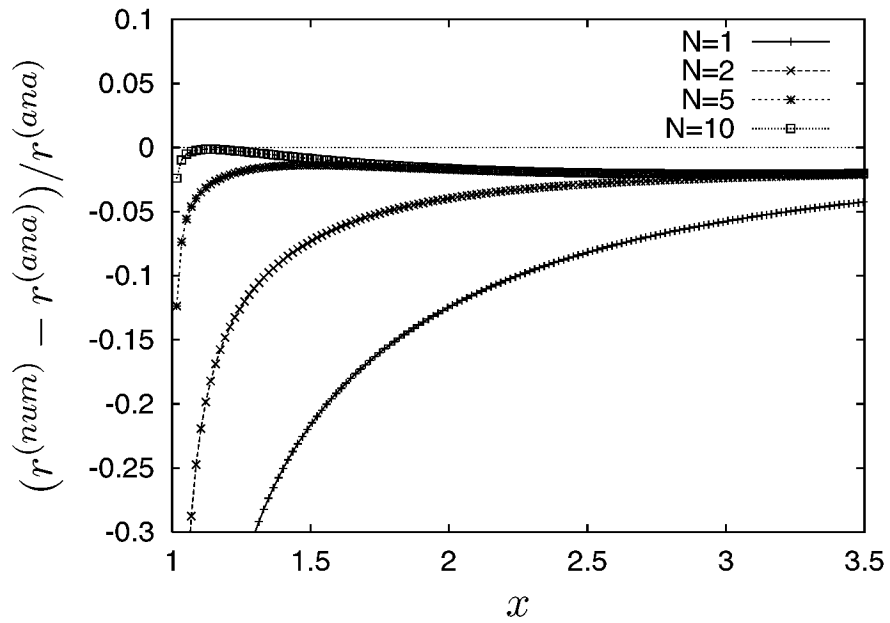


Figure 7.8: Comparison of the of the numerical value of $r = \sigma_{xx}/\sigma_{yy}$ with its analytical prediction along the x -axis in front of the crack. If more modes of expansion are used, then the deviation of the theoretical value form its analytical expectation becomes closer to zero.

As a test scenario, we use a parabolic crack, as depicted in Fig. 7.5 and given by the relation $2x + y^2 = 2$. The value of the residuum and the effective driving force depend on the number of expansion modes. The results are shown in Fig. 7.6 for different propagation velocities³. The residuum initially decreases very fast by inclusion of a few modes but seems to saturate at a finite level which depends on the velocity. We clearly see that only for low velocities the driving force Δ does not differ too much from the effective value Δ_{eff} . This indicates that this method to solve the elastic problem is not very suitable for all velocities. Furthermore, the results depend on the “length” of the crack; formally, we always deal with semi-infinite crack, but for the numerical reasons we have to cut the shape at a certain distance from the tip. The dependence of the residuum and the effective driving force on this tail cut point x_{tail} is shown in Fig. 7.7. As result, all values have almost reached their limiting value as soon as the total length of the crack has exceeded several tip radii.

For the static case, the analytic solution of the parabolic crack is known; in particular, the stresses in front of the crack, $y = 0$ are at distances $x - 1 \ll 1$ from the tip [44]

$$\sigma_{xx} \sim \left[\frac{1}{(x - 1/2)^{1/2}} + \frac{1}{2} \frac{1}{(x - 1/2)^{3/2}} + \mathcal{O}((x - 1/2)^{-5/2}) \right], \quad (7.72)$$

$$\sigma_{yy} \sim \left[\frac{1}{(x - 1/2)^{1/2}} + \frac{1}{2} \frac{1}{(x - 1/2)^{3/2}} + \mathcal{O}((x - 1/2)^{-5/2}) \right]. \quad (7.73)$$

The ratio is

$$r := \frac{\sigma_{xx}}{\sigma_{yy}} = \frac{x - 1}{x}. \quad (7.74)$$

In Fig 7.8 the deviation of the numerical value from the analytical prediction is shown. We clearly see that the agreement becomes very good by introduction of more modes.

We also checked the numerical procedure using other crack shapes like in Fig. 7.9. The convergence is very similar to the parabolic crack and only for low velocities we obtain really convincing results.

The solution of the elastic problem by series expansion requires introduction of an origin of the stress field singularities. Nevertheless, the physical properties should be independent of the choice of this origin. Of course, this can be fulfilled only in the limit $N \rightarrow \infty$. However, we can see that shifting the origin by Δx does not lead to strong variations of the effective driving force for relatively low propagation velocities (see Fig. 7.10); again the results are less good for higher speeds.

In summary, we see that the developed expansion technique to solve elastodynamic crack problems gives good results for relatively low velocities $v \ll v_R$, but becomes worse for higher velocities.

7.2.5 Summary

In this subchapter we developed a method to solve steady state elastodynamic crack problems for arbitrary shapes in the tip region. We use an expansion of the singular part of the elastic fields in a set of eigenmodes of a straight mathematical cut. Far away from the tip, the stress field exhibits the normal $r^{-1/2}$ decay.

We also examined more carefully the relation between the dynamic and the static stress intensity factor. Only the latter one is an experimentally directly controllable parameter

³The propagation velocity is prescribed and not determined by the surface diffusion process.

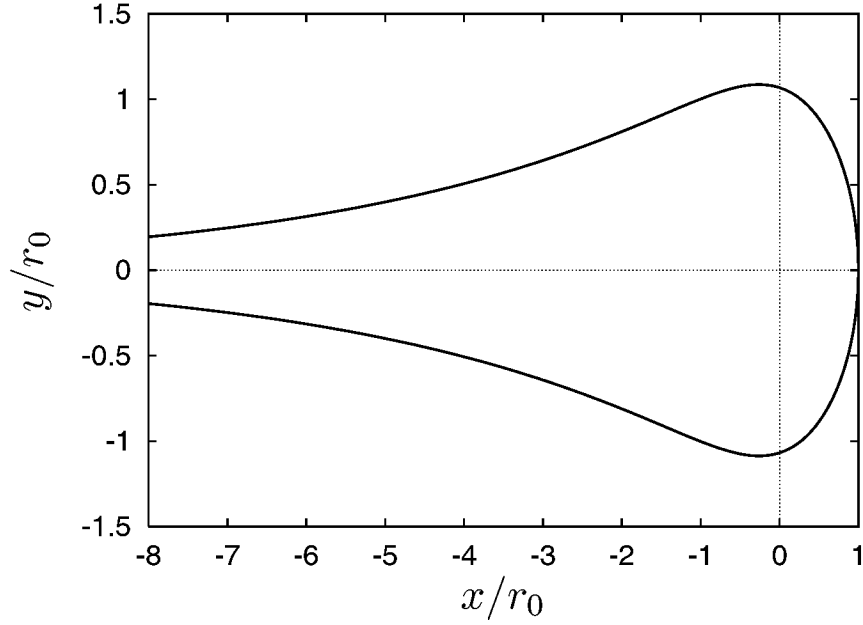


Figure 7.9: Crack shape which is used to solve the elastic problem with the expansion technique. In particular, the independence on the choice of the origin of the eigenmodes can be checked.

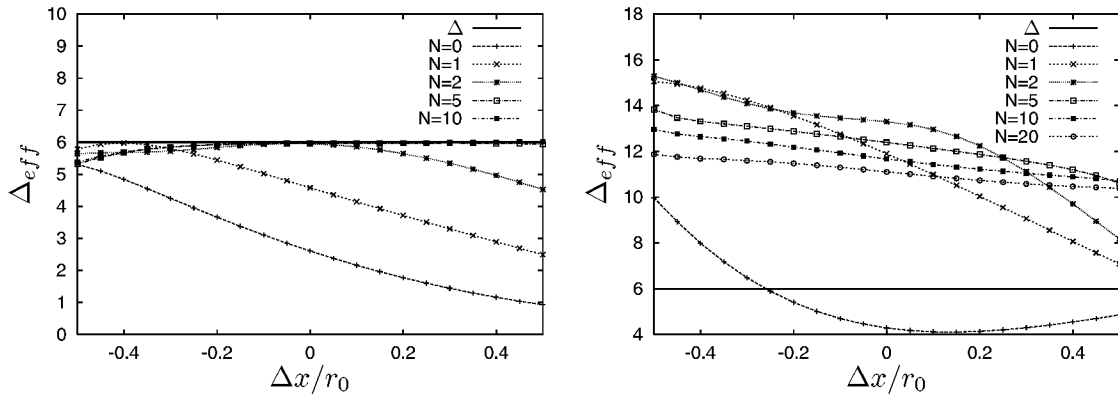


Figure 7.10: Dependence of the effective driving force on the choice of origin for the shape in Fig. 7.9. The more modes we include, the less sensitive are the results. $\Delta = 6$ is the driving force. In the left graph, the propagation velocity is $v = 0.1548 v_R$, in the right one $v = 0.9506 v_R$. Though the effective driving force does not depend too strongly on the shift of the origin for a more accurate series, the deviation from the real driving force Δ is very serious for the higher propagation velocity.

of the system. The relation between both of them depends either on the the propagation velocity and the geometry of the torn solid. In order to allow steady state growth, we study a semi-infinite crack in a narrow strip.

Finally, we solved different test scenarios, using the developed methods. It turns out that convergence towards the exact solution is rather good for low propagation velocities but becomes worse if it approaches the Rayleigh speed.

7.3 The forward integration method

In this section we present a numerical method which enables us to find steady state solutions for a growing crack. Primarily, this method is of course designed for surface diffusion as a mass transport mechanism, but it can also be used for melting-recrystallization processes. The latter is important for many experimental realizations of the Grinfeld instability, but turns out to be important for metallurgical processes as well. We will discuss this specific application in the next section; here we describe the numerical methods. We also present two important tests, the evolution of a hole in a solid which deforms by surface diffusion without elastic influence, and also the local crack model of section 6.3.1.

For the numerical evaluation of the local model, we transformed the steady state equation of motion into a (nonlinear) third order differential equation. This was possible, because the stress was a pure local quantity which, at a certain point of the crack surface, does not depend on the entire shape. Tip radius and propagation velocity are selected by the required fulfillment of boundary conditions either at the tip and in the tail region of the crack. Already here the dependence of the solution of the differential equation was very sensitive against changes of the boundary conditions. They are applied at different end points of integration, and we used a shooting method to determine the parameters above [58]. However, the dependence of the solution on these parameters turned out to be very sensitive, and consequently it was rather difficult to find good guesses for the shooting parameters. Only finally the results were very robust, when already good initial guesses were known.

A similar approach can in principle be used for the full solution of the elastodynamic problem: Effectively, the stress is now a non-local property of the crack, and therefore the equation for the steady state shape becomes also nonlocal. Nevertheless, by the use of a relaxation technique, it can be transformed into an iteratively improving sequence of differential equations: One starts with an initial guess for the crack shape and also an initial guess for the propagation velocity. For this configuration one solves the elastodynamic problem by series expansion and determines the coefficients of the higher modes. For *fixed* coefficients, one can in principle solve now the corresponding (local) third order differential equation. Then one obtains a new shape and a new crack speed, which differs from the original guesses. Here it becomes already obvious that this leads to an iterative procedure, since one can redo the calculations with the obtained data as new input. Unfortunately, this method, which should find all information self-consistently, turns out to be unstable. Extended simulations never led to a convergent result.

Thus we developed a different technique, which has already been used successfully for dendritic growth [31, 61, 62]. In contrast to the former approach, we do not search explicitly for steady state solutions but start with an arbitrary crack shape. Then we really perform a time-dependent simulation of crack propagation (by surface diffusion or melting and recrystallization); knowing that a stable steady state solution should exist at least below a critical value of the driving force, the idea is that the crack shape finally converges towards this configuration. Then we can use the current propagation velocity as good approximation for its steady state value. Since we do not rescale the equation of motion to a dimensionless form,

we can finally measure the tip radius of the crack.

We call this approach the *forward integration method*, because we use for simplicity an explicit Euler scheme for integration of the equation of motion [58]. The disadvantage of this technique is that the timesteps have to be very small, because otherwise the algorithm becomes numerically unstable. We will comment on this problem in the next section. The computation time for reasonably fine grids gets easily too long, and therefore it will be unavoidable to implement an implicit scheme in the future. However, this is a major project due to the nonlinearity of the problem.

We discretize the shape by a set of points, define normal vectors and curvature. Also, we calculate the stress fields at each interface point and are thus able to determine the chemical potential. The flux of material to the neighboring “atoms” is proportional to the tangential derivative of the chemical potential, and the local normal velocity is given by the equation of motion (6.7). We use this information to displace each interface point in normal direction at each timestep Δt ; for a growing crack, this shifts the whole crack in positive x direction. Since we are interested in the steady state shape, given in a co-moving frame of reference, we move the whole crack back such that the crack tip is always located at a desired position. If the point density becomes too high or low, we remove or insert points. This guarantees not only a smooth interface discretization but assures also numerical stability which depends on the point separation $ds = (dx^2 + dy^2)^{1/2}$.

Concerning the solution of the elastodynamic problem we remark that we do not solve it exactly for the transient stage when shape and velocity still change, but assume that it is currently in steady-state. This means that this relaxation regime is not handled exactly, only the final solution is correct and fulfills the fundamental equations.

Technically, the developed program performs the following steps after initialization, i.e. discretization of the initial shape by a set of points (x_i, y_i) :

1. Calculate the “geometrical” information: separation of neighboring points, curvature, normal vectors.
2. Add or remove points if the point density becomes too high or too low.
3. Adjust the boundary conditions. E.g. for a “surface diffusion crack”, tail points are added according to an exponential decay; it is assured that the tip is located at positions $x = 1/\kappa(\text{tip})$, as described in section 6.3.1. Another example is a closed hole in a solid (see next section): Here “periodicity” requires that the last point is at the same position as the first one.
4. Assume that the crack moves in steady state with the current “pseudo steady state velocity” v . Solve the elastodynamic problem as described in section 7.2.2. Calculate the expansion coefficients. Usually, it is not necessary to perform this time consuming step with each run of the main loop, since the crack shape does not change very much.
5. Calculate the chemical potential μ at each surface point.
6. Compute the normal velocity v_n at each surface point. For melting and recrystallization $v_n \sim \mu$, for surface diffusion $v_n \sim \partial^2 \mu / \partial t^2$.
7. Advance each interface point by $v_n \Delta t$ in normal direction.

8. Determine the next pseudo steady state velocity according to the differential equation

$$\frac{dv}{dt} = \frac{v_n(tip) - v}{\tau_0}, \quad (7.75)$$

with a suitably selected relaxation timescale τ_0 . This avoids dramatic changes of the velocity in subsequent steps. Also, it prevents from velocity overshoots, i.e. transient velocities which exceed the Rayleigh speed and forbid solution of the elastodynamic problem. In steady state, the velocity must always be subsonic. In the limit $\tau_0 \rightarrow 0$ we have an instantaneous adjustment of v to the tip velocity. In all other cases, this is valid only after relaxation.

9. Shift back all points in negative x direction such that the tip always remains at the well-defined position $x = 1/\kappa(tip)$. Thus, we describe the crack effectively in a co-moving frame of reference.

10. back to step 1.

7.3.1 Surface diffusion driven by curvature

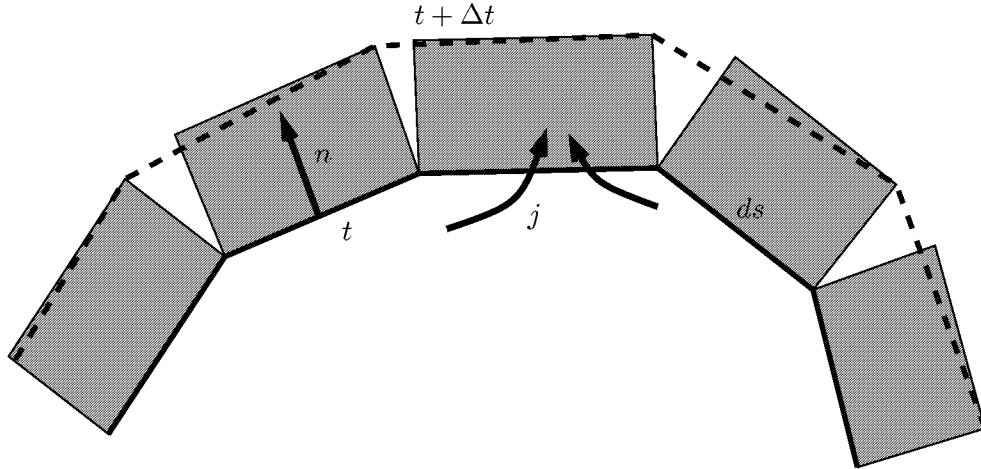


Figure 7.11: The timestep Δt leads to an advance of the interface. The interface at time t is depicted by the solid line, at $t + \Delta t$ by the dashed line. Volume conservation is not exactly fulfilled since the volume between the interface contours does not exactly match the volume inside the rectangular boxes. Their volume is determined by the total incoming flux j within the time interval Δt and leads to a normal shift of the interface.

The first test of the procedure described above is to study the evolution of a hole inside a solid, arising from surface diffusion which is driven by surface energy alone and does not take elastic effects into consideration. We expect that this hole deforms to a circle of the same area.

The underlying equation of motion conserves by construction the volume of the body. In principle, we have to assure that this is also fulfilled by our numerical procedure. However, the discretization of space and time which we use does not exactly conserve the volume: The

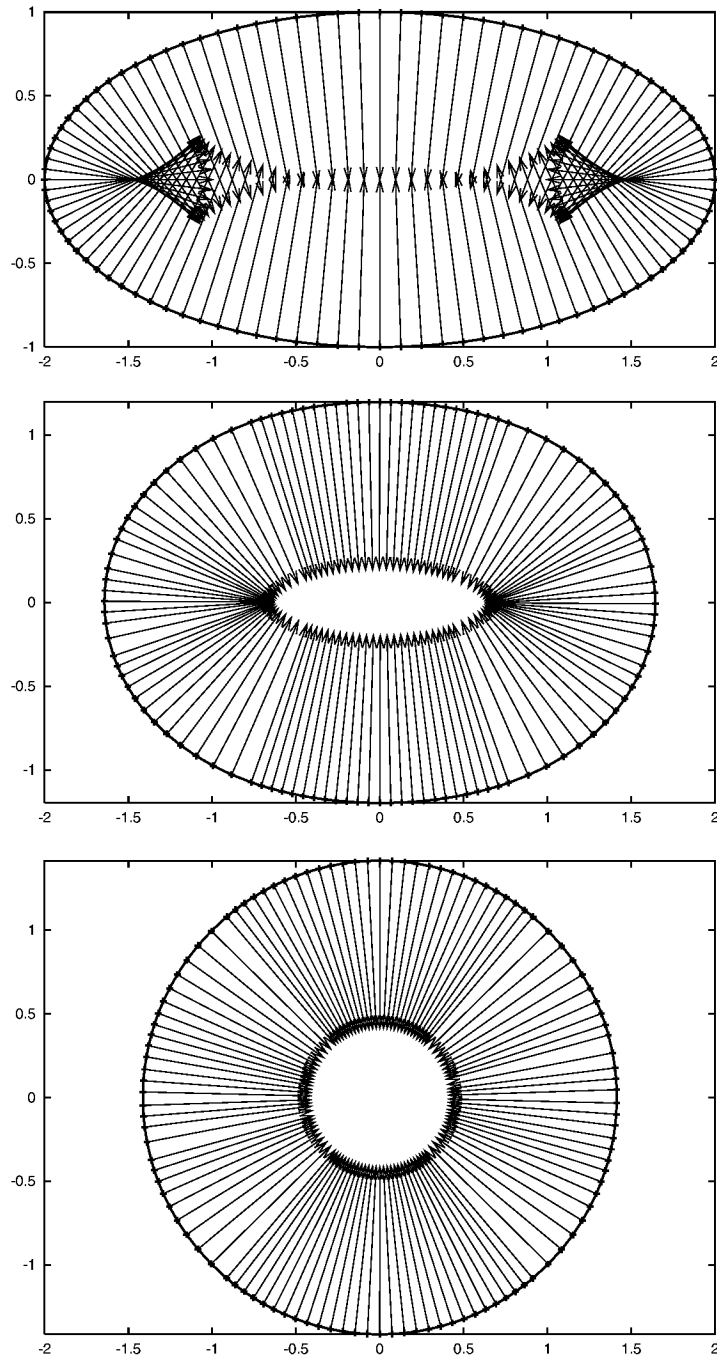


Figure 7.12: The initial ellipse deforms more and more towards the final circle. The second profile is at $t = 0.3$, the third at $t = 10$. All contours are drawn together with normal vectors.

general procedure is (see Fig. 7.11) that we calculate the total flux of material into a certain line element. The advance in *normal* direction is such that the totally accumulated material during a timestep Δt is stored in a rectangle above this line element. This defines a procedure how to shift the interface points. Thus the solid contour of the body is shifted to the new (dashed) one. Geometrically, the volume between the two contours differs from the volume inside the rectangles for finite timesteps Δt . Therefore, volume conservation is only valid up to $\mathcal{O}(\Delta t^2)$. To second order, this difference is $\delta V \sim \kappa ds (v_n \Delta t)^2$ for one length element ds , in comparison to the rectangular volume $V \sim ds v_n \Delta t$.

This curvature correction turns out to be not very important, which can be understood best from the equation of motion for an almost flat interface in (x, y) representation

$$\dot{y} = -Dy'''''. \quad (7.76)$$

Analytically, this equation is always stable, i.e., a perturbation of the initially flat surface $y_0(x, t) \equiv 0$ by $\delta y = \exp(ikx + \lambda t)$ has a stable spectrum $\lambda = -Dk^4$. A numerical discretization $y(j\Delta x, n\Delta t) = y_j^{(n)}$ with the usual representation of derivatives, e.g. $y'_{j+1/2} = \frac{1}{\Delta x} [y_{j+1}^{(n)} - y_j^{(n)}]$ leads to the von Neumann stability condition [58]

$$\Delta t < \frac{(\Delta x)^4}{8D}, \quad (7.77)$$

if we assume a perturbation $y_j^{(n)} = \xi^n \exp(ikj\Delta x)$. This means that we have to choose the timestep Δt rather small. The second order correction mentioned above is therefore not important.

To check the numerical code, we consider an elliptical hole and neglect all elastic effects. Thus only the curvature drives an interface flux which finally deforms the ellipse to a circular hole (see Fig. 7.12). After each timestep the density of interface points is checked and eventually adjusted; too big separations between points reduce the accuracy of the calculation whereas too small gaps make the forward scheme unstable according to Eq. (7.77). This is cured by an automatic adding or removing of interface points. The boundary conditions of a continuously closed shape and flux conservation are fulfilled by periodic continuation of the shape. In dimensionless units ($D = 1$), we discretize the ellipse with semiaxes $a = 2, b = 1$ by 100 interface points. The chosen timestep is $\Delta t = 1e^{-6}$, and the program assures that the distance between neighboring points is always between $s_{min} = 0.06$ and $s_{max} = 0.12$. Volume conservation turns indeed out to be fulfilled very well: From the initial ellipse to the final circle in Fig. 7.12 the relative change of the total volume is about 10^{-4} without curvature correction.

In conclusion, the forward integration method works well for surface diffusion processes. We illustrated that an elliptical hole deforms, as expected, to a circle. Unfortunately, the timesteps have to be selected to be very small in order to avoid numerical instabilities.

7.3.2 The local model

We used the forward scheme also to verify the results which we obtained from the steady state calculations for the local stress model (6.10). It turns out that the initial shape is not very important and finally always converges to the steady state shape that we obtained already earlier (see Fig. 7.13).

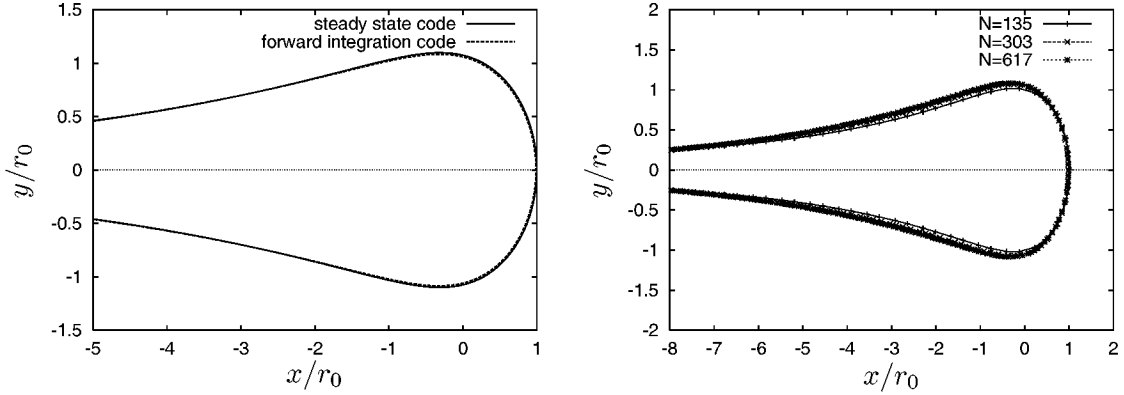


Figure 7.13: Comparison of the crack shapes from the steady state code and the forward scheme (left). The driving force is $\Delta = 1.21$. In the latter case we used 617 abutments to discretize the crack shape. The tip radius is $r_0 = 0.31(D/v_R)^{1/3}$ and the propagation velocity $v = 0.328 v_R$. Both curves are almost indistinguishable. Convergence of the crack shapes for different numbers of interface points N (right). The resulting tip radii of curvature are $r_0^{(135)} = 0.4(D/v_R)^{1/3}$, $r_0^{(303)} = 0.325(D/v_R)^{1/3}$ and $r_0^{(617)} = 0.31(D/v_R)^{1/3}$.

The crack shapes for different point densities are also given in Fig. 7.13. Though for low grid point densities the tip radius still depends on the discretization, the shapes are already very close to the final shape.

For the propagation velocity, which enters into the expression of the elastic field, we do not use the actual tip velocity $v(\text{tip})$ but the artificial velocity v which obeys the differential equation

$$\frac{dv}{dt} = \frac{v(\text{tip}) - v}{\tau_0}. \quad (7.78)$$

Typically, we use the timescale $\tau_0 = 1D^{1/3}v_R^{-4/3}$. As soon as we have reached the steady state configuration, we have $v = v(\text{tip})$. This procedure avoids strong fluctuation during the initial stage when the solution has not yet converged towards the final steady state and makes the numerical code stable. Also, the non-steady propagation velocity can crucially exceed the Rayleigh speed or become even negative.

At each timestep we calculate the normal shift of each interface point; afterwards, the whole crack is shifted back such that the tip point is always located at $x = r_0$, in agreement with the local model of section 6.3.2. Therefore, effectively the grid points wander along the interface towards the tail, since we apply the diffusion equation in the laboratory frame of reference. Consequently, the grid thins out in the tip region, and from time to time we have to insert new grid points there if their density becomes too low. As a result, this leads to a modification of the shape in the tip region and causes jumps in the actual propagation velocity and tip radius. However, this effect becomes obviously less pronounced if we use a higher point density. Then the oscillation frequency of the velocity and the tip radius becomes higher (since the insertion of points happens more often) and simultaneously the amplitude decreases (see. Fig. 7.14).

With increasing number of grid points the agreement with the steady state calculations becomes better and better (see Fig. 7.15).

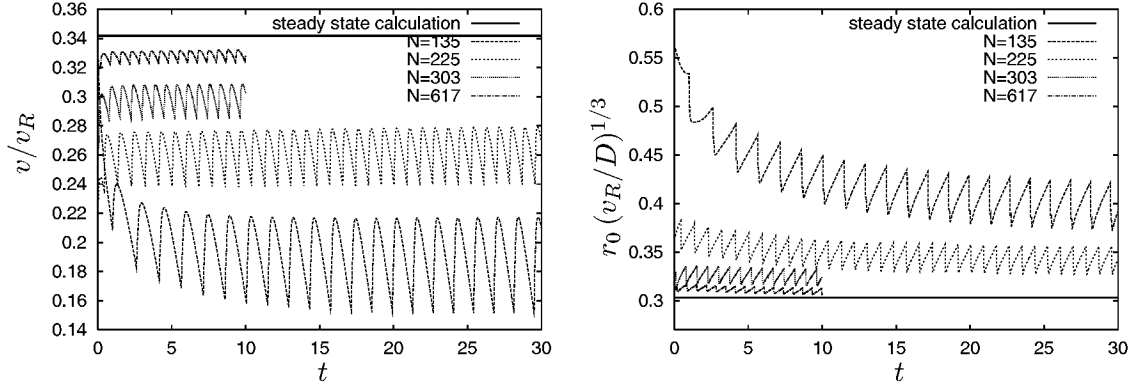


Figure 7.14: Convergence of the velocity (left) and the tip radius (right) towards its steady state value for $\Delta = 1.21$. We always use the relaxed shape for the next calculation with more grid points N . The frequency of the velocity fluctuations increases with the number of grid points, whereas its amplitude becomes smaller. The calculations with the higher point densities were stopped earlier, since the steady state regime was already reached.

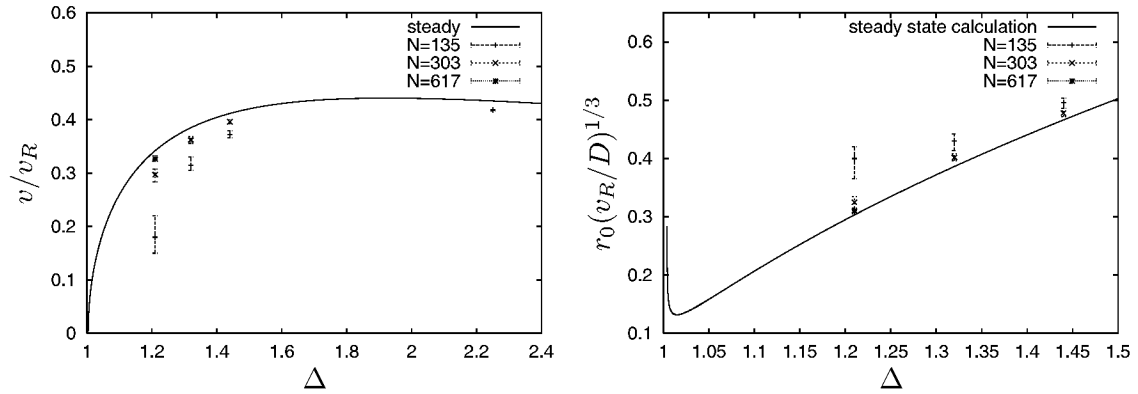


Figure 7.15: Comparison of the propagation velocity (left) and the tip radius (radius), calculated by the steady state method with the forward integration method. With more grid points N to discretize the crack shape the agreement between both approaches becomes obvious. Here we show only for a few specific values of the driving force how the quality of solution improves with the grid resolution.

In summary, we applied the forward integration method to the local crack model of section 6.3.2 and obtained a good agreement of the results for calculations with higher accuracy. This confirms the former results and opens a new approach to solve complicated crack problems which go beyond the local model.

7.3.3 Summary

The *forward integration method* which we described in this subchapter together with some numerical tests, is the last ingredient for a numerical realization of the full problem of fast crack growth by surface diffusion. We implemented and checked this routine, verified in particular the numerical volume conservation for the deformation of a circular hole in a solid material. As a next step, we reproduced the results which we obtained already earlier for fast crack propagation with the local stress model. The calculations give independent evidence to the former results.

The central problem of the current implementation is that it uses for simplicity an explicit Euler scheme for integration of the equations of motion. For a surface diffusion process, this limits the maximum timestep Δt to $\Delta t \sim (\Delta s)^4$ with the point separation Δs , which dramatically slows down the process. It will be unavoidable to implement an (at least partially) implicit scheme in the future, because for the current code the computation times can become too long for reasonable calculations.

7.4 The melt finger

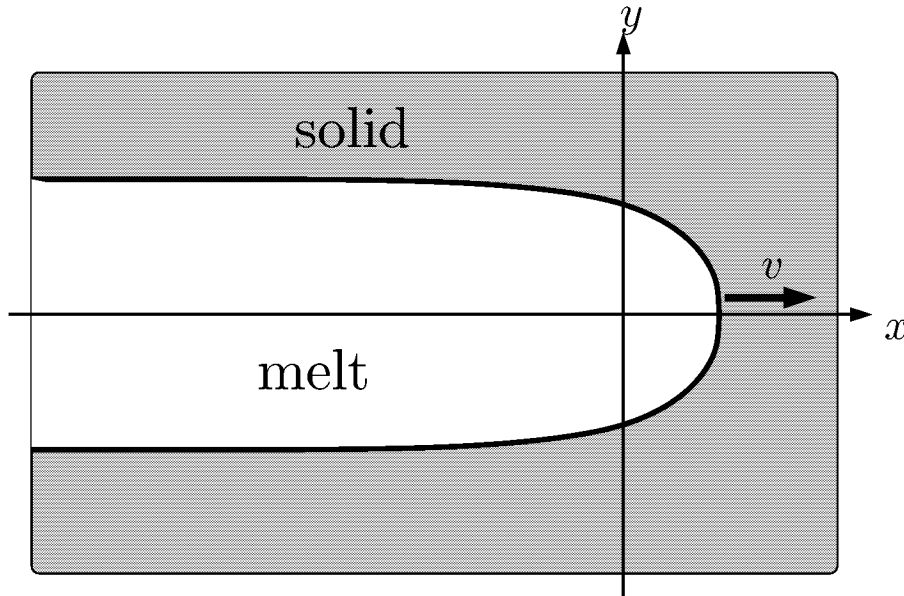


Figure 7.16: Expected shape of a growing melt finger in a channel.

In chapter 4 we studied the coarsening of melt inclusions inside a overheated solid. We pointed out that the elastic deformation due to the density difference leads to important

modifications of the coarsening dynamics and the shape of the inclusions. These inclusions are lentil-like and have many similarities with cracks.

Now we refrain from the complicated interactions between neighboring inclusions but study the detailed dynamics near the tip of the inclusions. Instead of surface diffusion as driving dynamics we have now a melting and recrystallization of the phases; the amount of each phase is not conserved separately. In chapter 4, stresses arose due to density differences. Here we apply an external stress. Again, a nonhydrostatic loading leads to the Grinfeld instability. The deep notches are comparable to a semi-infinite crack in a narrow channel.

We have to adopt the general counting arguments, which we used in the previous chapter to describe crack propagation, to this new scenario. One very important observation is that there is no need for the (undeformed) “melt finger” to close far away from the tip since we do not have to obey a material conservation law (see Fig. 7.16).

The equation of motion reads now in comparison to Eq. (6.7)

$$v_n = \frac{D_{mc}}{\alpha\Omega}\mu, \quad (7.79)$$

with the kinetic coefficient of the melting-recrystallization transition D_{mc} , which has dimension $[D_{mc}] = \text{m}^2\text{s}^{-1}$.

In the tail region all elastic fields have decayed and the equation of motion therefore is

$$\dot{y} = D_{mc}y''. \quad (7.80)$$

For steady state growth, we have

$$-vy' = D_{mc}y'', \quad (7.81)$$

with the general solution

$$y(x) = A + Be^{-vx/D_{mc}}. \quad (7.82)$$

Here we cannot neglect the constant contributions which is forbidden in the crack problem by volume conservation. The growing exponential (the tail is oriented towards $x \rightarrow -\infty$) has to be suppressed by proper selection of the propagation velocity. Therefore the final shape is expected to look like Fig. 7.16.

Again, we study the limit of high propagation velocities; the Rayleigh speed sets an upper limit. We do not rescale the equation of motion by the tip radius of curvature r_0 , since this is not an adjustable parameter here; Eq. (7.79) is only a second order equation, and therefore we cannot prescribe the tip radius, since the curvature is determined by the equation of motion and not by boundary conditions. Instead, we use the opening A for a dimensionless rescaling. We define the dimensionless length scales and velocities

$$\tilde{x} = x/A, \quad \tilde{v} = vA/D_{mc}. \quad (7.83)$$

The dimensionless chemical potential reads

$$\tilde{\mu} = \frac{A}{\alpha\Omega}\mu. \quad (7.84)$$

Then the equation of motion becomes simply

$$\tilde{v}_n = \tilde{\mu}, \quad (7.85)$$

and the tail behavior is

$$\tilde{y} = 1 + \tilde{B}e^{-\tilde{v}\tilde{x}}. \quad (7.86)$$

The boundary condition at the tail is $\tilde{B} = 0$, i.e. suppression of the growing exponential. We locate the tip at the arbitrary position⁴ $\tilde{r}(\theta = 0) = \tilde{r}_0/2$; symmetry requires $\tilde{r}'(\theta = 0) = 0$.

The counting procedure is now very similar to the crack problem: Imagine to start integration at the tip; then we have to kill the growing exponential at the tail and also assure that the constant opening is indeed $\tilde{y} = 1$. Therefore we need two parameters. Again, the lengthscale A has dropped out of the equations and cannot provide a selection. Therefore, we need two parameters, $\tilde{v}$ and v/v_R . Here again the inertial effects are necessary.

We use again the local model (6.10) for the stress field. The results for the propagation velocity and the tip radius are given in Fig. 7.17.

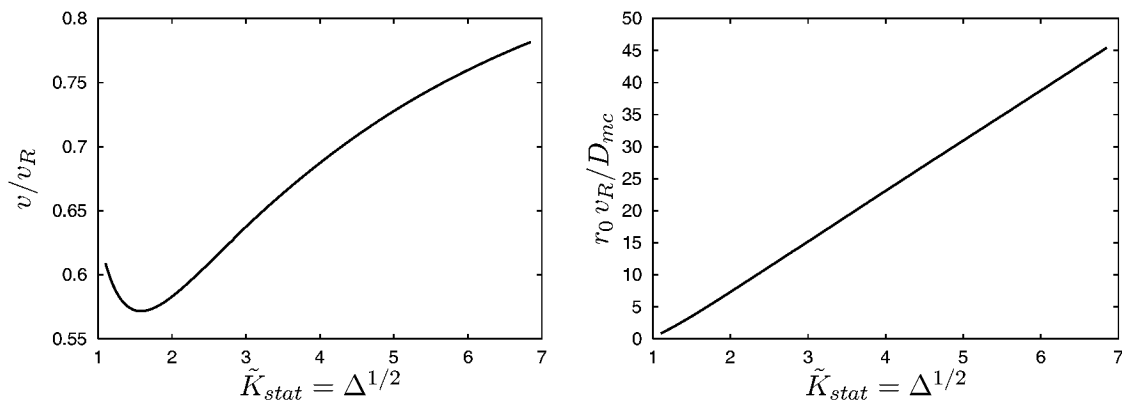


Figure 7.17: Propagation velocity (left) and tip radius (right) versus (dimensionless) static stress intensity factor in the framework of the local stress model. Only the branch of high velocities is physical, but might be screened by the Grinfeld instability.

Again, we expect the occurrence of the Grinfeld instability for higher driving forces, if we take into account the complete and nonlocal elastic field.

Two corresponding steady state shapes are given in Fig. 7.18. They look indeed as expected, only for higher velocities the shift of the maximum tangential stress to other angles than $\theta = 0$ leads to the formation of two “sidebranches”. It is quite conceivable that the Grinfeld instability pronounces this effect and leads to a real tip-splitting.

If we do not take the inertial terms into account, i.e. $v_R \rightarrow \infty$ in (6.10), then a steady state solution does not exist, in agreement with our counting arguments. No explicit lengthscale appears in this problem, and by reducing the scale arbitrary L , the propagation velocity increases, whereas the tip radius decreases as function of time and would finally reach zero if it was not cut off by the grid spacing (see Fig. 7.19 and 7.20).

7.4.1 Numerical results

The main advantage of the melt crack in comparison to the crack growth by surface diffusion is that the underlying equation of motion is of second instead of fourth order. This allows

⁴In *principle*, this choice is irrelevant, but it turns out that the local model is unstable if we select e.g. $\tilde{r}(\theta = 0) = \tilde{r}_0$.

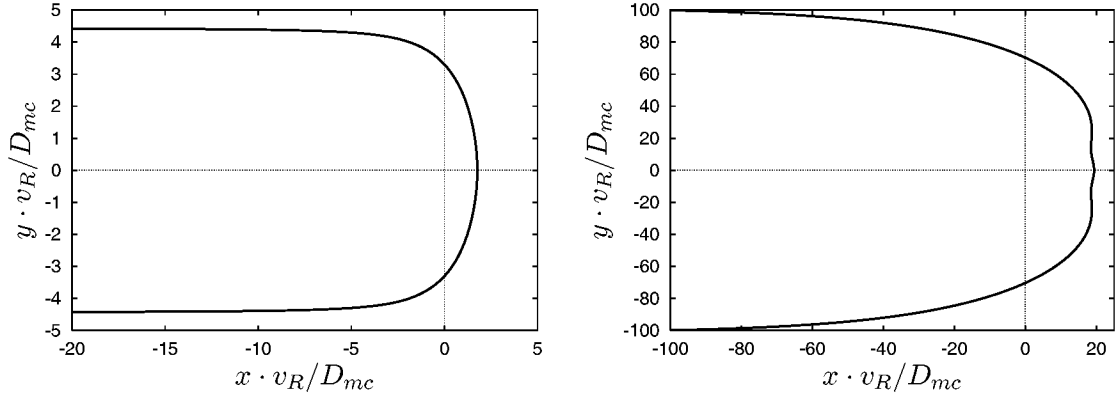


Figure 7.18: Steady state shape of a melt crack for $\tilde{K}_{stat} = \Delta^{1/2} = 1.5$ (left) and $\tilde{K}_{stat} = \Delta^{1/2} = 6$ (right) in the framework of the local stress model.

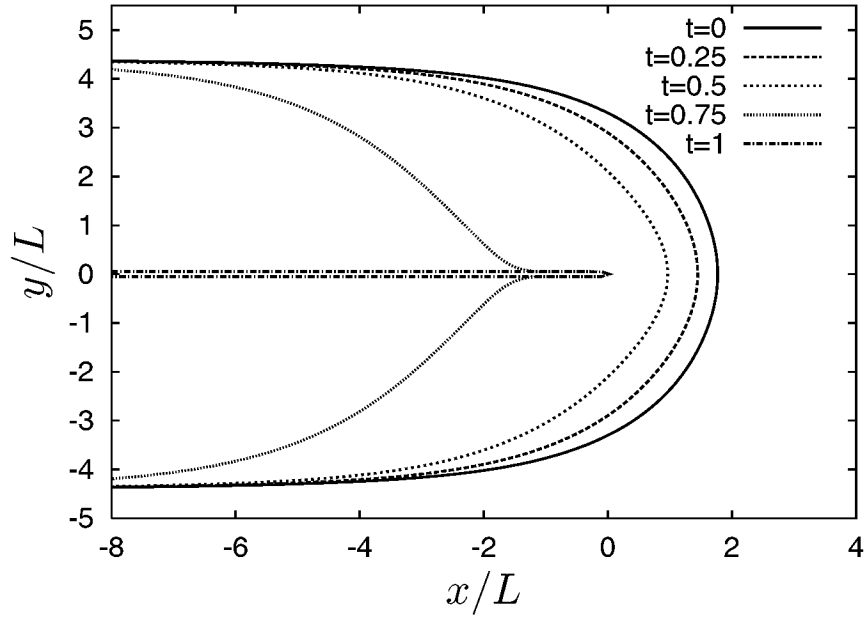


Figure 7.19: Evolution of an initial shape without inertial effects. The tip radius decreases and the cusp singularity is cut off only by the grid resolution. An intrinsic lengthscale is not present in this problem, therefore the shape is given on the arbitrary lengthscale L . The unit of time is L^2/D_{mc} . We use the relaxation law (7.78) with timescale $\tau_0 = 1$.

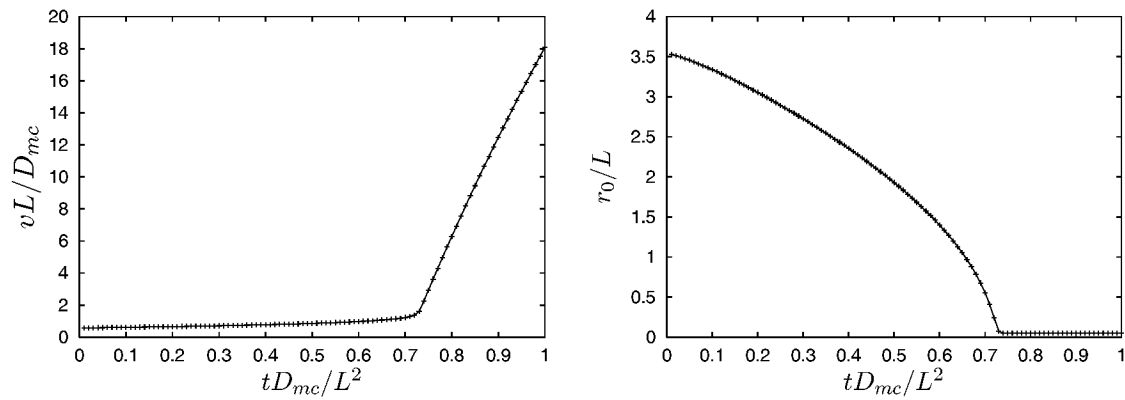


Figure 7.20: Evolution of propagation velocity and tip radius as function of time. The cusp singularity becomes obvious. The lengthscale L is arbitrary and not selected by the equations.

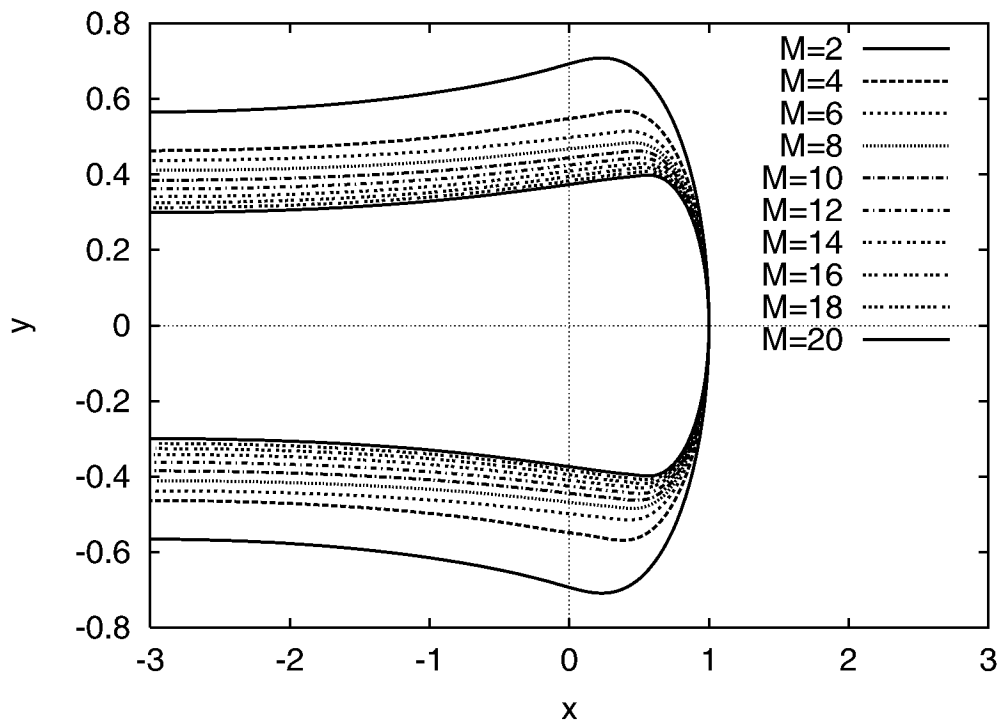


Figure 7.21: Improvement of solution of the full problem for growth of a melt finger in a channel. M denotes the number of expansion modes.

bigger timesteps $dt \sim (ds)^2$ and therefore much faster computations.

Here we present some first results of the full problem, including solution of the elastodynamic equations. We use the near tip expansion technique of section 7.2, together with the exact boundary conditions as derived in section 7.1.

However, it does not make sense to include too many modes: high frequency modes with big values $-n$ in (7.48) and (7.49) cannot be represented on a coarse grid with spacing ds ; at a typical distance R from the origin, the characteristic angular distance between neighboring points is $d\theta \sim ds/R$. Oscillations of the sin and cos terms must be representable on this scale, therefore we require $1/|n| \gg d\theta$. Typically, for objects of scale $R \approx 1$ in dimensionless units, we use $ds \sim 0.05$ for a fine representation of the shape. The above criterion tells us that it is definitely not very reasonable to use modes with n bigger than 10.

The choice of the origin of the stress field expansion should in principle be irrelevant in the limit of an infinite number of modes. Though it can be chosen arbitrarily, it would be the best idea not to set it explicitly, but to relate it to another scale in the system, which should come out self-consistently. Similarly to the former calculations, it would be reasonable to set $x(\text{tip}) = Cr_0$ with the distance of the tip to the origin $x(\text{tip})$, the tip radius r_0 and a fixed number C of order unity. However, it turns out that this approach is unstable, and therefore we have to set $x(\text{tip})$ explicitly. The hope is, that finally for an increasing number of modes, the precise choice of the origin is irrelevant and leads only to an overall translation of the crack. This tendency should become more pronounced if the number of modes is increased. However, our present results do not obey this property yet, and further investigations are necessary. It seems that the choice of origin influences the intrinsic lengthscales of the system, whereas the propagation velocity does not change very much. We believe that this is due to the current non-fulfillment of the boundary conditions with sufficient precision.

A preliminary sequence of steady state shapes of melt fingers is shown in Fig. 7.21. Here we really solve the elastic problem by series expansion with more and more expansion modes. It will be a major task for the future to check and improve the quality of these time-dependent calculations.

7.5 Summary

In this chapter we refined the simplified version of crack growth by surface diffusion to the full problem which contains all effects. This includes a modification of the expression for the chemical potential and the elastic boundary conditions in order to take into consideration all inertial effects. We also designed a numerical method to solve the multiscale elastodynamic problem of a steady crack with arbitrary shape in the tip region. Using an expansion technique in eigenfunctions of a straight cut, we do not have to solve the elastic equations everywhere in the bulk but just have to fulfill the boundary conditions; this reduces the numerical efforts drastically. Together with the *forward integration method* to find steady state configurations by integration of the equations of motion, we provide all necessary tools to solve the full problem of fast crack growth by surface diffusion.

Since this problem is very hard to solve, we started with the simpler and related task to describe the growth of a melt finger in a channel subjected to an external loading. We used the forward integration method not only together with the local stress model, but also with the expansion technique for the real solution of the elastodynamic problem. Finally, we presented preliminary results, but a complete evaluation will be a major task for the future.

Chapter 8

Summary

The general aim of this thesis was to analyze the influence of elastic effects on segregation, and to possibly transfer results onto fracture processes. We found several important links between these different fields of research, and by combining them we gained completely new insights. In particular, the nucleus of a first order phase transition in an elastic medium corresponds to a Griffith crack. The Grinfeld instability, driven either by surface diffusion or by melting and recrystallization was found to be an important connection. It leads to morphological deformations of elastically strained interfaces. On the one hand, it opens a consistent approach to understand the influence of elastic effects on phase transformations, on the other hand, its deep notches, developing in the late stage of the instability, exhibit clear relationships to fast growing cracks.

The Grinfeld instability is based on a competition between a release of elastic energy and an increase of surface energy. Since the full thermodynamic equilibrium is not reached here, a precise differentiation between surface energy and surface tension has to be made. The first step was to study the additional influence of surface tension on the Grinfeld instability. We derived the modified spectrum of the stability analysis for a uniaxially strained planar surface subject to surface diffusion. Although the modifications due to surface tension are usually negligible, we discovered a destabilization even without an external uniaxial force resulting from self-stresses. More importantly, we found a strategy to derive a consistent set of equations for our model using variational principles; this enabled us to deduce these equations through simple physical reasoning, and thus they can easily be generalized.

During a melting process, stresses can appear not only due to external forces, concentration and temperature gradients, but also due to density differences between the solid and liquid phases. We discussed the coarsening regime of melt inclusions inside a superheated solid phase. Elastic effects lead to oblatelly shaped inclusions, resulting in a system with strong diffusional and elastic interactions between them. We found that the usual mean-field description by Lifshitz, Slyozov and Wagner breaks down and several independent length scales have to be taken into account. In a system of parallel inclusions, we also found the scaling laws for the coarsening of the different length scales involved. In particular, the lateral size of the precipitates obeys a nontrivial growth law, $R \sim t^{5/12}$, which differs systematically from the classical growth exponent $1/3$. This leads to a decay of the excess temperature and to the final equilibrium state of the system. In consequence, previous experiments on coarsening in solids possibly should be reanalyzed with respect to the scaling exponent.

A closely related problem is the growth of cracks in a uniaxially strained solid. Provided

that one can ignore finite size effects, several cracks appear in the sample and lead to a relaxation of stresses. Situations like this can often be observed in geological systems, such as earthquakes, but also in experiments at the laboratory scale. A strong interplay between neighboring cracks lets the longer cracks grow at the expense of the shorter ones; this is similar to a conventional coarsening process. Here, however, the full fractal hierarchy of crack lengths can remain if a receding crack is hampered by surface oxidation. Both processes, the coarsening of cracks and the melting of a superheated solid, have many properties in common: The overall stress relaxes similarly to the excess heat of the overheated uniaxial solid. Further, the elastic tension can in both cases be projected onto the bending of thin plates between neighboring cracks or melt inclusions. This clearly shows the similarities of fracture processes and coarsening kinetics with elastic effects. We were able to analytically derive the scaling laws for the growth of the relevant lengthscales and the decay of the stresses. We found that the average length of the cracks grows according to the coarsening law $R \sim t$ with the highest possible exponent in dissipative systems. The vertical separation of the cracks scales as $\ell \sim t^{4/5}$, and the remaining stress in the system, which is analogous to the overheating in a solid, scales as $P \sim t^{-4/5}$.

So far, a linear phenomenological law was used to relate the crack speed to the energy release rate. However, crack propagation exhibits several peculiarities for higher propagation velocities. Thus, we studied in a next step the growth of a single crack in more detail, concentrating on the dynamics in the tip region. We present a continuum theory which describes the fast growth of a crack by surface diffusion. The basic idea arose when trying to remove the unphysical cusp singularity of the Grinfeld instability. The deep notches which appear in the late stage of this process are comparable to fast growing cracks. By introducing a fully dynamical theory of elasticity, it was possible to produce a self-consistent selection of the crack tip radius. This theory describes the complicated dynamics of a crack tip, the elastic far field behavior, and the deformation of already existing cracks. To the best of our knowledge, this is the first time this has been done in a simple and controlled manner, without introduction of complicated theories of plasticity, which are not yet fully developed.

Our theory predicts — in agreement with experimental observations — the saturation of the steady state crack velocity appreciably below the Rayleigh speed, and the blunting of the crack tip. Though surface diffusion is commonly believed to be slow, it can lead to fast crack propagation: the velocity is on the scale of the Rayleigh speed. The reason for this unexpected behavior is that even in the framework of our purely macroscopic continuum theory using typical material parameters, the tip radius is on the atomic scale, and therefore the transport length for surface diffusion is very small. Furthermore, our model includes the possibility of a tip-splitting instability for high applied tensions. In particular, we introduced a local stress model which covers the essential features of the real elastic fields. It was used to outline the fundamental ideas and calculate the tip velocity, tip radius and the crack shape in the tip region. The local model itself is not unstable against a secondary Grinfeld instability; we checked this in a tedious numerical calculation and by analytical arguments. However, nonlocal effects in a full description can indeed cause a tip-splitting instability.

Finally, we went beyond the local model and extended the concept of fast crack propagation to a complete description. This requires the evaluation of the fully dynamical chemical potential as driving force for the surface diffusion process and a numerical solution of the elastodynamic equations applied to the real steady state crack shape. Following a procedure similar to the derivation of the Grinfeld instability with surface tension, we deduced the equations of motion, the corrected boundary condition and the modified chemical potential, now

consistently taking inertial effects into account. We developed a numerical method to solve elastodynamic steady state problems of growing cracks of arbitrary shapes, by using a series expansion in terms of the eigenfunctions of a semi-infinite straight crack with a sharp tip. The advantage of this procedure is that it allows us to calculate all the stress components in the tip region, only requiring the compliance with the boundary conditions, and without having to solve the elastic bulk equations. We developed a program which reduces this task to the problem of minimization of a functional, and solved it numerically. Several tests have shown that the quality of the solution improves with increasing number of expansion modes. For propagation velocities sufficiently below the Rayleigh limit, the developed technique matches analytical predictions for static cracks.

A simple forward integration scheme allows us to find steady state solutions of crack growth. We showed that without elastic effects, an elliptical hole in a solid deforms, as expected, to a circle. Furthermore, we applied this numerical method to our local stress model and confirmed the previous results.

A problem that is closely related to the crack propagation by surface diffusion, is the growth of a melt finger in a stressed channel. In a similar way as for crack growth, we derived the selection mechanism for the propagation velocity and the tip radius. We used the local stress model to compute quantitative predictions in the regime of fast growth. Finally, we presented results for the full problem, including an exact solution of the elastic problem. Though these results are preliminary and still are lacking somewhat in numerical precision, they form an encouraging basis for further development. These methods also seem to offer a promising approach for solving the challenging problem of fast crack propagation by surface diffusion without further approximations, including a numerical prediction of the tip-splitting instability.

Appendix A

Derivation of the steady state equation

Here we give a derivation of Eq. (6.8) which is used in chapter 6.3.1.

Surface diffusion provides an expression for the local propagation velocity of an interface point. Usually, the interface moves in a complicated way, and only under certain circumstances a steady-state evolution, where the shape of the interface is preserved in a co-moving frame of reference, is possible. Here we derive an equation for the interface shape which obeys this steady state propagation.

The shape is given by a function $y(x, t)$ or $r(\theta, t)$. The cartesian shape is given in the laboratory frame of reference, the polar description in a moving frame of reference with velocity v (motion in x direction), which, at the moment is not restricted to be constant. Later, we will apply the general results to the special case of steady state motion. The transition between both descriptions given by (see Fig. A.1)

$$x = r \cos \theta + vt, \quad (\text{A.1})$$

$$y = r \sin \theta. \quad (\text{A.2})$$

Now we also look at a specific point on the interface. By surface diffusion, individual atoms move *along* the interface, driven by the chemical potential μ with a flux $j \sim d\mu/d\tau$, where τ denotes the tangential coordinate. The interface itself moves in *normal* direction, described by the diffusion equation

$$v_n = -\frac{D}{\alpha\Omega} \left(\frac{\partial^2 \mu}{\partial \tau^2} \right)_{n,\tau}, \quad (\text{A.3})$$

where D is the surface diffusion coefficient, α the surface energy density and Ω the atomic volume. This equation is valid in the laboratory frame of reference. The motion of the specific point $x_0(t), y_0(t)$, describes the motion of an interface point and not of an atom. We therefore obtain the cartesian equations of motion

$$\frac{dx_0}{dt} = \dot{x}_0 = -\frac{y'}{\sqrt{1+y'^2}} v_n, \quad (\text{A.4})$$

$$\frac{dy_0}{dt} = \dot{y}_0 = \frac{1}{\sqrt{1+y'^2}} v_n, \quad (\text{A.5})$$

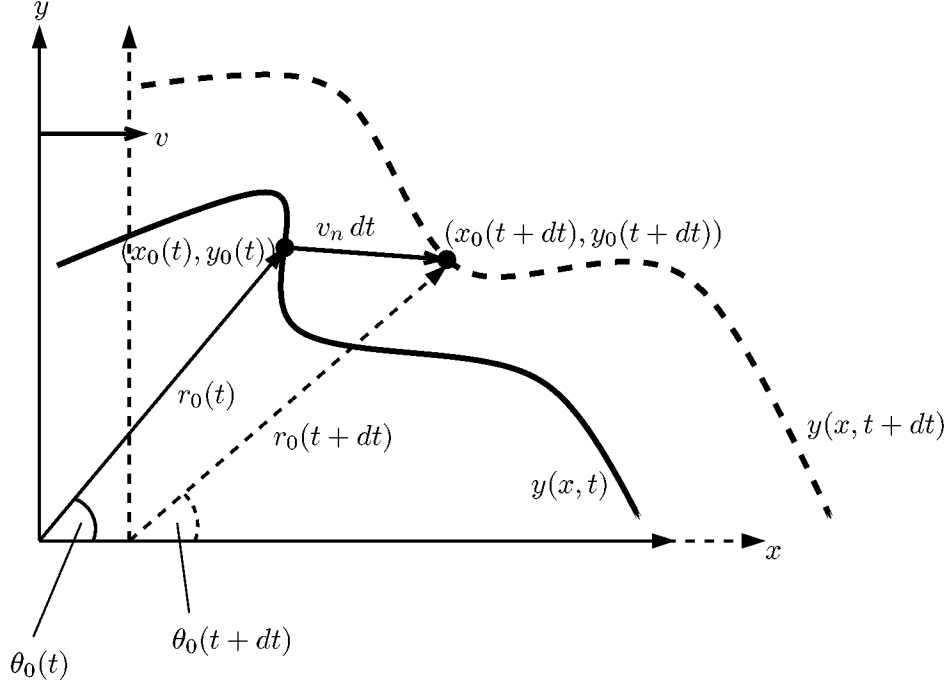


Figure A.1: Evolution of an interface. The solid lines correspond to time t , the dashed curves to $t + dt$. Atoms diffuse along the surface, which itself moves in normal direction.

where the prime denotes the partial derivative with respect to x ,

$$y' = \frac{\partial y(x, t)}{\partial x}. \quad (\text{A.6})$$

The second derivative of the chemical potential is given in polar coordinates by

$$\left(\frac{\partial^2 \mu}{\partial \tau^2} \right)_{n,t} = \frac{1}{\sqrt{r^2 + r'^2}} \left(\frac{\partial}{\partial \theta} \right)_t \left[\frac{1}{\sqrt{r^2 + r'^2}} \left(\frac{\partial \mu}{\partial \theta} \right)_t \right]. \quad (\text{A.7})$$

From Eqs. (A.1) and (A.2) follows readily

$$y' = \frac{r' \sin \theta + r \cos \theta}{r' \cos \theta - r \sin \theta} \quad (\text{A.8})$$

with

$$r' = \frac{\partial r(\theta, t)}{\partial \theta}. \quad (\text{A.9})$$

The point $(x_0(t), y_0(t))$ or $(\theta_0(t), r_0(t))$ is always located on the surface. Therefore

$$r(\theta(t), t) = r_0(t), \quad (\text{A.10})$$

and consequently

$$\dot{r}_0 = r' \dot{\theta}_0 + \dot{r}. \quad (\text{A.11})$$

Using the polar equations of motion, which follow from (A.1) and (A.2),

$$\dot{r}_0 = (\dot{x}_0 - v) \cos \theta + \dot{y}_0 \sin \theta \quad (\text{A.12})$$

$$\dot{\theta}_0 = \frac{\dot{y}_0 \cos \theta - \dot{x}_0 \sin \theta + v \sin \theta}{r} \quad (\text{A.13})$$

we get from Eq. (A.11)

$$\dot{x}_0 \left[\cos \theta + \frac{r'}{r} \sin \theta \right] + \dot{y}_0 \left[\sin \theta - \frac{r'}{r} \cos \theta \right] = \dot{r} + v \left(\frac{r'}{r} \sin \theta + \cos \theta \right) \quad (\text{A.14})$$

We can simplify this expression using (A.4) and (A.5) and gain

$$\sqrt{r^2 + r'^2} v_n = r \dot{r} + v(r' \sin \theta + r \cos \theta). \quad (\text{A.15})$$

This finally leads to the general equation of motion for the shape in polar coordinates

$$-\frac{D}{\alpha \Omega} \left(\frac{\partial}{\partial \theta} \right)_t \left[\frac{1}{\sqrt{r^2 + r'^2}} \left(\frac{\partial \mu}{\partial \theta} \right)_t \right] = r \dot{r} + v(r' \sin \theta + r \cos \theta) \quad (\text{A.16})$$

In the special case of steady state motion, $\dot{r} = 0$ in a co-moving frame of reference. Then the preceding equation can be integrated once (we assume the integration constant to be zero) and obtain

$$\frac{D}{\alpha \Omega} \frac{1}{\sqrt{r_s^2 + r_s'^2}} \left(\frac{\partial \mu}{\partial \theta} \right)_t = -v r_s \sin \theta, \quad (\text{A.17})$$

where $r_s(\theta)$ denotes the steady state shape. In cartesian, now also co-moving coordinates, this equation reads

$$\frac{D}{\alpha \Omega} \frac{1}{(1 + y_s'^2)^{1/2}} \left(\frac{\partial \mu}{\partial x} \right)_t = v y_s \quad (\text{A.18})$$

as differential equation for the steady state shape $y_s(x)$.

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