

14. Juli 2003

1 Literaturübersicht zum Projekt Halbleiter, JIFF08

Projektleiter: Prof. Kurt Schroeder

(Akkumulierte Liste seit April 1998)

1. K. Schroeder, S. Blügel, B. Engels, P. Richard, "Reexchange controlled Diffusion in Surfactant-mediated Epitaxial Growth: Si on As-terminated Si(111)", Phys. Rev. Lett. 80, 2873 (1998)
2. B.Engels, P.Richard, K.Schroeder, S.Blügel, Ph.Ebert, K.Urban, "Comparison between *ab initio* theory and scanning tunneling microscopy for (110) surfaces of III-V semiconductors", Phys.Rev. B 58 (12), 7799 - 7815 (1998)
3. R.Berger, S. Blügel, A. Antons, Wi. Kromen, K. Schroeder: "A Parallelized *ab initio* Molecular Dynamics Code for the Investigation of Atomistic Growth Processes", Proceedings of the NIC-Workshop "Molecular Dynamics on parallel Computers", Jülich, 08.-10. Februar 1999, p. 185-198 (World Scientific 2000)
4. K.Schroeder, A. Antons, R.Berger, Wi. Kromen, S. Blügel: "Surface Diffusion and Models for the Kinetics of Epitaxial Growth", Proceedings of the International Symposium on Structure and Dynamics of Heterogeneous Systems, held at Duisburg, 25.-26. Februar 1999, p. 71-94 (World Scientific 2000)
5. R. Spettmann, P.Entel, K.Schroeder, S. Blügel: "Elektronic Structure of Si(111):Sb ($\sqrt{3} \times \sqrt{3}$) R30⁰: an *ab initio* Study", Proceedings of the International Symposium on Structure and Dynamics of Heterogeneous Systems, held at Duisburg, 25.-26. Februar 1999, p. 217-225 (World Scientific 2000)
6. A. Settels, Schroeder, K.; Korhonen, T.; Papanikolaou, N.; Aretz, M.; Zeller, R.; Dederichs, P.H.: "In-donor complexes in Si and Ge: structure and electric field gradients", Solid State Communications 113, 239 (2000)
7. K.Schroeder, A. Antons, R.Berger, S. Blügel: "Ad-Atom Kinetics on Surfactant-covered Si(111), *ab initio* Calculations", International Symposium on Structure and Dynamics of Heterogeneous Sytems, Duisburg, Germany, 28-29 August 2000. Phase Transitions 75, 91-99 Part A (Jan-Feb 2002).
8. K.Schroeder, A. Antons, R.Berger, S. Blügel: "Surfactant mediated heteroepitaxy versus homoepitaxy: Kinetics of group-IV atoms on As-passivated Si(111) and Ge(111)", Phys. Rev. Lett. 88, 046101 (2002) (28. January 2002).
9. Yi-gang Cao, Jiao Zheng-Kuan, A. Antons, K. Schroeder, and S. Blügel, "Stable Structure of Sb Monolayer on a Strained Ge(111) Substrate", Chin. Phys. Lett. 19, 259 (2002) (02. February 2002).

10. Yi-gang Cao, Jiao Zheng-Kuan, A. Antons, K. Schroeder, and S. Blügel, "Relaxation of Small Molecules, an *ab initio* Study", Comm. Theor. Phys. (China) 37, 597 (2002) (15. May 2002).
11. A. Hirnet, K. Schroeder, S. Blügel, X. Torrelles, M. Albrecht, B. Jenichen, M. Gierer, W. Moritz, "A novel Sb induced reconstruction of the (113) surface of Ge", Phys. Rev. Lett. 88, 226102 (2002) (03. June 2002).
12. A. Antons, K. Schroeder, B. Voigtländer, V. Cherepanov, R. Berger, S. Blügel, "Element Specific Surface Reconstructions of Islands During Surfactant-Mediated Growth on Si(111)", Phys. Rev. Lett. 89, 236101 (2002) (18. Nov. 2002).
13. A. Antons, Y. Cao, B. Voigtländer, K. Schroeder, R. Berger, S. Blügel, "Strain-induced surface structures on Sb-covered Ge(111): Epitaxial Ge film growth on Si(111):Sb" Europhys. Lett., Vol. 62 (No.4) p. 547-553 (May 15, 2003).
14. Kurt Schroeder, Armin Antons, Bert Voigtländer, "Surfactant-Mediated Epitaxy" in "CNI - The Center of Nanoelectronic Systems for Information Technology", Chr. Buchal (Ed.), p. 20-27 (Forschungszentrum Jülich, May 2003)
15. A. Antons, K. Schroeder, "Group-IV adatoms on Surfactant-terminated Si(111): Diffusion, Incorporation and Clustering", Review article for Research Signpost, accepted May 2002.
16. A. Hirnet, K. Schroeder, W. Moritz, "Understanding of adsorption kinetics and equilibrium structure at surfaces: Sb on Ge(113)", in preparation.
17. A. Antons, R. Berger, B. Voigtländer, K. Schroeder, "Structure of step edges on As-covered Si(111): *ab initio* calculations and STM-images", in preparation.

2 Diplom- und Doktorarbeiten der Gruppe Schroeder

(Akkumulierte Liste seit April 1998)

1. Diedrich Frielinghaus, "ab initio Berechnungen von BeSe und BeTe (100)-Oberflächen", Diplomarbeit RWTH Aachen, 1998
2. Winfried Kromen: "Die Projector Augmented Wave-Methode: Ein schnelles Allelektronenverfahren für die *ab initio* Molekulardynamik", Dissertation RWTH Aachen, Oktober 2000
3. Armin Antons: "First-Principles Investigation of Initial Stages of Surfactant Mediated Growth on the Si(111) Substrate", Dissertation RWTH Aachen, Juli 2001
4. Ralf Berger: "Berechnung der Stufenkanten auf der As-bedeckten Si(111)-Oberfläche mit einem parallelisierten *ab initio* Programm", Dissertation RWTH Aachen, Juli 2002