Electrical properties of rolled-up p-type Si/SiGe heterostructures

N. V. Demarina and D. A. Grützmacher

Articles you may be interested in

Electrical and optical properties of p-type InGaN
Appl. Phys. Lett. **95**, 261904 (2009); 10.1063/1.3279149

Simulation of hole phonon-velocity in strained Si/SiGe metal-oxide-semiconductor transistor
J. Appl. Phys. **95**, 713 (2004); 10.1063/1.1633346

Extremely high room-temperature two-dimensional hole gas mobility in Ge/Si 0.33 Ge 0.67 /Si(001) p-type modulation-doped heterostructures
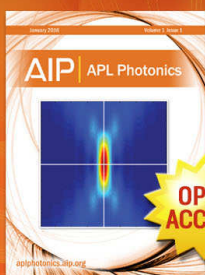Appl. Phys. Lett. **80**, 3117 (2002); 10.1063/1.1473690

Electrical depth profile of p-type GaAs/Ga(As,N)/GaAs heterostructures determined by capacitance–voltage measurements
J. Appl. Phys. **88**, 4153 (2000); 10.1063/1.1290449

Influence of technological parameters on the behavior of the hole effective mass in SiGe structures
J. Appl. Phys. **88**, 1978 (2000); 10.1063/1.1304839

Electrical properties of rolled-up p-type Si/SiGe heterostructures

N. V. Demarina[a)] and D. A. Grützmacher

Institute for Semiconductor Nanoelectronics, Peter Grünberg Institute-9, Forschungszentrum Jülich, D-52425 Jülich, Germany and Jülich-Aachen Research Alliance-Fundamentals of Future Information Technology (JARA-FIT), Germany

We report a theoretical study of the hole density and the low-field mobility in modulation p-doped rolled-up Si/SiGe heterostructures. Solving coupled Poisson and Schrödinger equations, we show that the total hole density is strongly affected by charged surface states and can reach value of 10^{11} cm^{-2} for available doping level at room and low temperature. The simulation of the hole transport along the structure axis based on a Monte Carlo method reveals that the interface roughness scattering is a main mechanism limiting the mobility magnitude, which reaches the value of 10^4 cm^2/V s. © *2011 American Institute of Physics*. [doi:10.1063/1.3584869]

On the evolutionary way toward nanoelectronics new functional devices made from nano-objects promise an exciting but challenging era as several key requirements should be met for large-scale manufacturing of those devices, among them controllability of all parameters, positioning capability with high precision, reliability, and effective cost. The potential ability of the semiconductor nano-objects can be substantially enhanced by introducing within them heterostructures.[1–3] The latter requirements can be elegantly fulfilled using the new technique based on the phenomenon of self-scrolling of a film comprising two strained semiconductor layers released from a semiconductor substrate.[4,5] Because of their high surface-to-volume ratio and tunable charge carrier transport properties due to quantum confinement effects electrical properties of rolled structures are strongly influenced by minor perturbations, which is especially apparent for use in electrical sensing devices as well as field-effect transistors. Further, the formation of tubes, rings, and coils achieved by releasing SiGe films opens ways to integrate these nano-objects into mature Si technology. While there exist numerous studies on magnetotransport of charge carriers in the tubes,[6–9] their electrical properties have not been yet considered sufficiently.[10] In this letter, we focus on the Si/SiGe rolled-up heterostructures grown on Si-substrate. In this type structures, band offset is mainly restricted to the valence band, making them useful for p-type devices. We theoretically analyze the influence of strain effect as well as charged surface states and doping level on the hole density in these structures. We also present a Monte Carlo study of the hole mobility in the rolled-up structures in low electric field parallel to the structure axis, which reveals impact of different scattering mechanisms on the drift mobility value and specifies the most important of them limiting the hole mobility in the structures

We consider a rolled-up structure reported recently in Ref. 11 formed from a bilayer consisting of Si and Si$_{1-x}$Ge$_x$ layers of h_{Si} and h_{SiGe} thickness, correspondingly, grown on (001) Si-substrate. In our theoretical treatment we assume that the structure is rolled into a single wall cylinder. The doping is applied to the layer of Si located at the inner surface of the tube with the width of 2 nm as it is shown in the inset of Fig. 1. This model of the doping approximately corresponds to the delta-doping of the original structure.

For the calculation of the hole density and mobility in the structure we first determine the strain in a stationary configuration of the tube making use of the linear elasticity theory,[12] which has been recently shown being a good approach and yielding results close to experimental data.[13,14]

The strain distribution strongly affects the electronic band structure.[15,16] First, we calculate the position of the conduction (E_{c0}) and valence (E_{v0}) band edges in rolled structures taking into account only the strain contribution to the band bending following the expressions from Ref. 17. The dash-dotted line in Fig. 1(a) shows the calculated position of the valence and conduction bands' edges for the Si/Si$_{0.2}$Ge$_{0.8}$ rolled structure. The band offset is mainly restricted to the valence band and the Si$_{0.2}$Ge$_{0.8}$ layer is a potential well for holes. Second, we take into account the additional electrostatic potential $V(r)$ due to the electric charge arising from modulation doping as well as the charged surface states
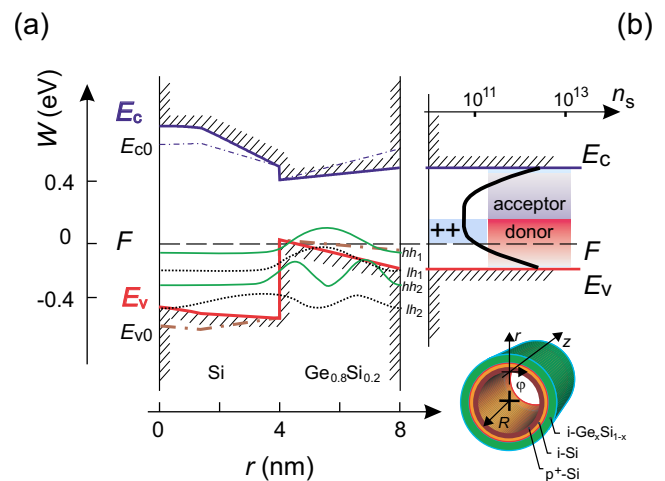

FIG. 1. (Color online) (a) Conduction (E_c) and valence (E_v) bands and Fermi level (F) in the Si/Si$_{0.2}$Ge$_{0.8}$ rolled structure calculated neglecting (thin dot-dashed line) and taking into account (thick line) the surface states and doping; shown are the moduli squared of the heavy-hole (solid line) and light-hole (dotted line) wave functions; (b) surface state density n_s at the SiO$_2$/p-Si interface; Inset: sketch of a rolled Si/SiGe heterostructure, which consists of Si and SiGe layers.

[a)]Permanent address: Radiophysics Faculty, Nizhniy Novgorod State University, 603950 Nizhniy Novgorod, Russia. Electronic mail: n.demarina@fz-juelich.de.

formed after the oxidation of the Si and Si$_{1-x}$Ge$_x$ surfaces. Therefore, the position of the conduction and valence bands fulfills $E_{c(v)} = E_{c(v)0} - qV(r)$, where q denotes the positive elementary charge. We find the electrostatic potential by the self-consistent solution of Poisson and Schrödinger equations, where the Schrödinger equation is solved for the envelope functions within the effective mass approach for heavy- and light-hole states assuming zero boundary conditions for the wave functions at the Si and SiGe surfaces. We note that for the typical layer thicknesses of the rolled structures, the radius exceeds 50 nm, which eliminates quantization of the hole spectrum for the momentum quantum number. As a result, the holes in the rolled-structures effectively form a two-dimensional hole gas. We integrate the Poisson equation neglecting the free electron charge and assuming that the doping atoms are fully ionized and the hole density is determined by the corresponding wave functions and occupation of the energy states. The total density of charged surface states at the inner surface determines the magnitude of the electric field normal to the surface, providing the boundary condition for the Poisson equation in the self-consistent cycle of the Schrödinger–Poisson solution. The full band bending is determined by the condition that the total space charge in a rolled structure matches the charge accumulated by surface states.

We describe the density of surface states on the inner and outer surfaces as a function of energy W by the U-type dependence, which for the (001) Si surface after oxidation at room temperature is presented in Ref. 18. We fit the experimental data with the following expression: $N_s(W) = A_{ns} \cosh\{B_{ns}(W - W_{mid})^2\}$, where W_{mid} denotes the energy of the middle of the gap, $A_{ns} = 5 \times 10^{11}$ cm^{-2} eV^{-1}, and $B_{ns} = 18$ eV^{-2}. Then, the Fermi level is pinned about 0.3 eV above the valence band edge at the Si$_{1-x}$Ge$_x$ surface for x = 0 and shifts toward the valence band with increasing Ge fraction for a total surface states density exceeding 5×10^{13} cm^{-2}, which is in agreement with the experimental data.[19]

The charge of the surface states depends on their position, the states lying above the middle of the gap are acceptor-type and below are donor-type. Figure 1(a) displays the calculated position of the bands at 4K for the Si/Si$_{0.2}$Ge$_{0.8}$ structure with a p-type Si layer (10^{12} cm^{-2}) and a total surface state density at each surface of 10^{12} cm^{-2}. The corresponding surface state density at the Si surface is presented in Fig. 1(b). Here, the Fermi level near the surfaces is approaching the valence band edge, leading to positive charge on both Si and SiGe interfaces. This, together with the modulation doping, gives rise to the downward tilt of the bands near the Si$_{0.2}$Ge$_{0.8}$ layer surface and the resulting accumulation of the hole gas at the Si/Si$_{0.2}$Ge$_{0.8}$ interface.

To reveal the influence of the surface states on the density of free holes in the channel, we vary the total surface state density by changing the coefficient A_{ns} within the 10^8–10^{12} cm^{-2} eV^{-1} range, without altering the qualitative shape of the surface state density function. We consider the Si and SiGe surfaces separately, first, increasing the density of surface states at the SiGe surface and assuming the Si surface to be ideal in the sense that the total surface state density is about 10^{10} cm^{-2}, and then vice versa.

Figure 2(a) shows the hole density in a structure composed of a 4 nm wide, p type (10^{12} cm^{-2}) Si layer and a 4
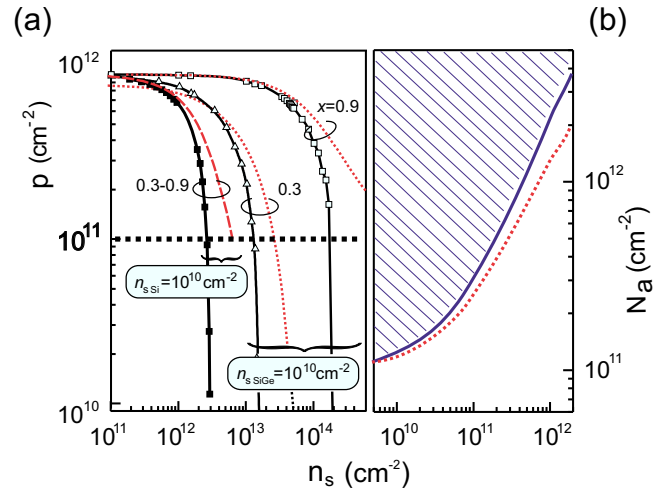

FIG. 2. (Color online) (a) Hole density in the Si$_{1-x}$Ge$_x$ layer vs the density of states on the Si$_{1-x}$Ge$_x$ and Si surfaces for different Ge content (x) in the Si$_{1-x}$Ge$_x$ layer calculated for low (4 K) (solid line) and room (300 K) (dashed and dotted lines) temperature; (b) the shaded area indicates the doping density of introduced acceptors in p$^+$-Si layer vs the density of states on the Si and Si$_{1-x}$Ge$_x$ surfaces in order to obtain the hole density in the SiGe layer above 10^{11} cm^{-2} for low (solid line) and room (dashed line) temperature.

nm wide SiGe layer. In accordance with the position of energy levels [Fig. 1(a)] the holes populate only the lowest energy state (hh1) both at low (4 K) and room (300 K) temperature. The hole density decreases first slowly and then rapidly with increasing surface state density, as more holes are trapped on the surface states. The surface states at the SiGe surface affect the hole density more strongly than those located at the Si surface. For the surface density of SiGe above 2×10^{12} cm^{-2}, the SiGe channel is depleted at low temperature and the rolled structure becomes nonconductive. For Si the surface state density might reach a value above 10^{13} cm^{-2} while the hole density remains above 10^{11} cm^{-2}. This we attribute to the close position of the Fermi level to the valence band edge at the surface of the SiGe layer, where the surface state density function rises more steeply than in the middle of the gap [Fig. 1(b)]. Due to the high fraction of ionized acceptor states at room temperature, the hole channel remains conductive up to high values of the surface state densities.

So far, we have discussed the hole density as a function of the surface state density while keeping the doping fixed. Now the minimal doping level to produce a conductive tube, having a hole density above 10^{11} cm^{-2} in the Si$_{1-x}$Ge$_x$ channel is calculated. Thus, we consider Si/Si$_{1-x}$Ge$_x$ rolled structures with x varying from 0.3 to 0.9 and the width of both layers varying from 2 to 12 nm. The layer thicknesses are restricted by the critical thickness for the growth of pseudomorphic strained layers.[17] We increase the total surface state density from 5×10^8 up to 10^{12} cm^{-2}, where the lower value corresponds to the surface, which is additionally passivated with hydrogen while the higher value describes a surface exposed to the oxidation in air at room temperature. We also assume that the density of states on SiGe surface is larger than on the Si surface by a factor of 5. The shaded area in Fig. 2(b) shows the doping density, which is required for a given surface state density to keep the hole density in the channel of the rolled structure above 10^{11} cm^{-2}. The calculation shows that the chosen density of the two-dimensional
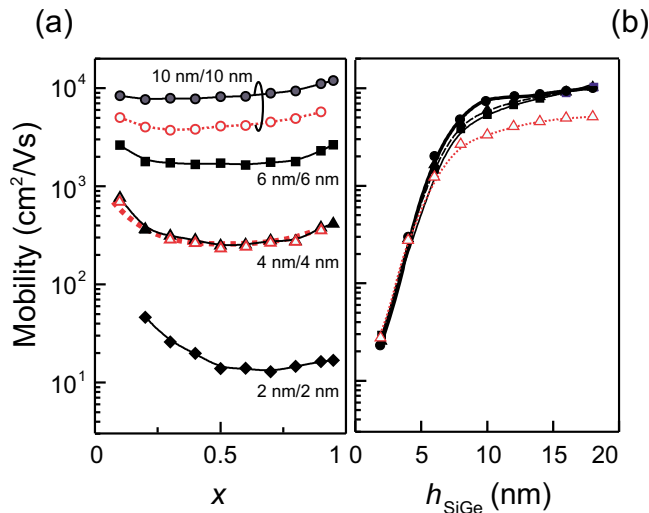
(a)   (b)

FIG. 3. (Color online) (a) Low-field hole mobility along the rolled structure axis as a function of Ge content x in the $Si_{1-x}Ge_x$ layer; the thicknesses of the Si and $Si_{1-x}Ge_x$ layers are equal and of 2, 4, 6, and 10 nm; (b) Low-field hole mobility along the $Si/Si_{0.5}Ge_{0.5}$ structure axis vs the $Si_{10.5}Ge_{0.5}$ layer thickness. The calculations are performed for low (solid lines) and room (dotted lines) temperature.

hole gas can be reached for any configuration of the tube within the defined limits by means available p-doping.

We calculate the low-field hole mobility in the rolled structures subject to a static electric field applied along the structure axis by means of the three-dimensional single-particle Monte Carlo method. We treat inelastic hole interplay with optical phonons and elastic interaction with acoustic phonons via deformation-potential coupling for bulk material.[20] We also take into account interface roughness scattering by using the scattering potential given by a δ-function at a perfect interface,[21] assuming that the interface exhibits small thickness fluctuation of 0.4 nm and the surface roughness correlation length in the direction parallel to the surface is about 2.5 nm.[22] We neglect hole scattering at the Si and SiGe surfaces as the hole gas is mainly confined in the vicinity of the Si/SiGe interface. The scattering rates for every structure are calculated numerically using the hole wave functions and energy levels obtained due to the solution of the coupled Poisson and Schrödinger equations.

In the transport simulations we assume that the surface state density at the surfaces is about 10^{10} cm^{-2} and choose the modulation doping to provide a hole density in the SiGe channel of 10^{11} cm^{-2}. Figure 3(a) shows the hole mobility as a function of Ge content in the $Si/Si_{1-x}Ge_x$ rolled structure with both layers set to thicknesses of 2, 4, 6, and 10 nm. The mobility dependence displays a pronounced minimum for a Ge content x ∼ 0.5. We attribute the decrease in mobility for $0 < x < 0.5$ to hole scattering by the Si/SiGe interface roughness, which dominates other scattering processes at low temperature and becomes stronger as the Ge content increases. Conversely, the substantial reduction in the hole effective mass in the SiGe layer with the larger Ge content ensures increasing mobility for $x > 0.5$. We note that the mobility also substantially drops with a decrease in layers thickness, which can be attributed to the stronger penetration of the hole wave function tail into the Si layer, leading to the stronger interplay between holes and the Si/SiGe interface imperfections. The presence of strong interface scattering in rolled structures with thin layers is also validated by the calculation

of the mobility at 300K [Fig. 3(a)]. In rolled structures with thick SiGe wells (above 8 nm), at 300K the holes are also effectively scattered by optical phonons, yielding a mobility lower than the low-temperature value by a factor of about 2. In structures with the narrow quantum wells, interface roughness scattering always dominates and makes the mobility temperature-independent.

Figure 3(b) shows that the low-field hole mobility increases with the width of the SiGe layer when the Si layer is set to 4 (squares), 6 (triangles), and 10 nm (circles). As discussed above, interface roughness scattering is reduced for wide SiGe layers causing a substantial increase in mobility from 20 to 10000 cm^2/V s. The width of the Si layer affects the mobility only slightly, as the holes are mainly confined to the SiGe layer. Comparison of the mobility calculated for 4 and 300K enables us to conclude that the optical phonon scattering affects hole transport in the rolled structures only if the SiGe layer thickness is larger than 5 nm.

In conclusion, the hole density in the rolled-up structures is strongly sensitive to the density of surface states; the additional strain introduced by the structure rolling-up does not lead to substantial enhancement of the hole mobility along the structure axis; however, further improvement might be expected for the hole mobility in the azimuth direction.

[1]F. Qian, Y. Li, S. Gradecak, D. Wang, C. J. Barrelet, and C. M. Lieber, Nano Lett. **4**, 1975 (2004).
[2]P. Mohan, J. Motohisa, and T. Fukui, Appl. Phys. Lett. **88**, 133105 (2006).
[3]A. Fontcuberta i Morral, D. Spirkoska, J. Arbiol, M. Heigoldt, J. R. Morante, and G. Abstreiter, Small **4**, 899 (2008).
[4]V. Y. Prinz, V. A. Seleznev, A. K. Gutakovsky, A. V. Chehovskiy, V. V. Preobrazhenskii, M. A. Putyato, and T. A. Gavrilova, Physica E (Amsterdam) **6**, 828 (2000).
[5]O. G. Schmidt and K. Eberl, Nature (London) **410**, 168 (2001).
[6]A. B. Vorob'ev, K.-J. Friedland, H. Kostial, R. Hey, U. Jan, F. Wiebicke, J. S. Yukecheva, and V. Y. Prinz, Phys. Rev. B **75**, 205309 (2007).
[7]N. Shaji, H. Qin, R. H. Blick, L. J. Klein, C. Deneke, and O. G. Schmidt, Appl. Phys. Lett. **90**, 042101 (2007).
[8]K.-J. Friedland, R. Hey, H. Kostial, A. Riedel, and K. H. Ploog, Phys. Rev. B **75**, 045347 (2007).
[9]C. Deneke, J. Schumann, R. Engelhard, J. Thomas, C. Muller, M. S. Khatri, A. Malachias, M. Weisser, T. H. Metzger, and O. G. Schmidt, Nanotechnology **20**, 045703 (2009).
[10]F. Cavallo, R. Songmuang, and O. G. Schmidt, Appl. Phys. Lett. **93**, 143113 (2008).
[11]Y. S. Yukecheva, G. Mussler, V. Shushunova, A. Weber, E. Deckardt, V. Y. Prinz, and D. Grützmacher, Semicond. Sci. Technol. **23**, 105007 (2008).
[12]M. Grundmann, Appl. Phys. Lett. **83**, 2444 (2003).
[13]B. Krause, C. Mocuta, T. H. Metzger, C. Deneke, and O. G. Schmidt, Phys. Rev. Lett. **96**, 165502 (2006).
[14]A. Malachias, C. Deneke, B. Krause, C. Mocuta, S. Kiravittaya, T. H. Metzger, and O. G. Schmidt, Phys. Rev. B **79**, 035301 (2009).
[15]S. Mendach, R. Songmuang, S. Kiravittaya, A. Rastelli, M. Benyoucef, and O. G. Schmidt, Appl. Phys. Lett. **88**, 111120 (2006).
[16]C. Ortix and J. van den Brink, Phys. Rev. B **81**, 165419 (2010).
[17]F. Schäffler, Semicond. Sci. Technol. **12**, 1515 (1997).
[18]M. H. White and J. R. Cricchi, IEEE Trans. Electron Devices **19**, 1280 (1972).
[19]R. L. Jiang, J. L. Liu, J. Li, Y. Shi, and Y. D. Zheng, Appl. Phys. Lett. **68**, 1123 (1996).
[20]K. Bhaumik, B. K. Ridley, and Y. Shacham-Diamand, J. Appl. Phys. **74**, 5546 (1993).
[21]G. Etemadi and J. F. Palmier, Solid State Commun. **86**, 739 (1993).
[22]S. Tsujino, C. Falub, E. Müller, M. Scheinert, L. Diehl, U. Gennser, and T. Fromherz, Appl. Phys. Lett. **84**, 2829 (2004).