Engineering self-assembled SiGe islands for robust electron confinement in Si

R. O. Rezaev,[1,2,*] S. Kiravittaya,[1] V. M. Fomin,[1] A. Rastelli,[1] and O. G. Schmidt[1]
[1]*Institute for Integrative Nanosciences, IFW Dresden, Helmholtzstr. 20, D-01069 Dresden, Germany*
[2]*Laboratory of Mathematical Physics, Tomsk Polytechnic University, Lenin Avenue 30, Tomsk 634050, Russia*
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The confinement potential and the energy of localized electron states in the Si matrix surrounding self-assembled SiGe/Si(001) islands are evaluated with realistic structural parameters. For homogeneously alloyed islands overgrown with Si at low substrate temperatures, a nonmonotonic dependence of the energy levels on size and composition is obtained and conditions to achieve the deepest confinement potential are derived within the available parameters. The influence of the experimentally reported composition distributions on the electron confinement is considered and confined states are found to lie as deep as 120 meV below the Si Δ conduction-band edge. Finally, shape changes occurring during Si capping at high substrate temperatures are shown to lead to a substantial reduction in the confinement potential. This work guides the design of structures able to provide robust single-electron confinement in Si.

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I. INTRODUCTION

A promising way to implement the idea of quantum computation in solid-state systems consists in considering the spin of electrons as a natural bit of quantum information.[1,2] Since the preservation of coherence is a basic requirement for this kind of application,[2–6] studies on mechanisms leading to an increase in spin lifetime and possibilities to control the state of a single spin are crucial. It has been shown that the strong confinement in low-dimensional structures, such as quantum dots (QDs), results in an increase in spin lifetime.[6–9] In silicon, three-dimensional (3D) confinement can be obtained by using electrons bound to single impurities[10] or by split gates applied to a two-dimensional electron gas defined at a SiGe/Si interface.[11–14] An alternative approach is represented by self-assembled SiGe/Si 3D islands which form during the epitaxial growth of a Ge film on a Si(001) substrate in the Stranski-Krastanow mode.[15–17] In the growth direction (z) the SiGe island creates, in fact, two quasitriangular potential wells for electrons in the Si matrix, one above and one below the island (Fig. 1) while in-plane localization is provided by the strain modulation in Si (see, e.g., Ref. 18). For isolated islands, the spread of strain in Si and, as a consequence, the energy of localized electron states are determined by the shape, size, and composition of the SiGe islands embedded in Si. In turn, the structural properties of the SiGe islands can be tuned by changing the growth conditions during Ge deposition and subsequent island capping with Si. In general, it is desirable to have QDs with strong confinement for a large energy separation between confined levels and to limit thermal escape of carriers. The latter is important for spin manipulation and leads to a reduction in spin dephasing associated with the spin-orbit coupling.[19] Furthermore, for experimental studies on confined electrons in QD ensembles based, e.g., on capacitance-voltage spectroscopy,[20] the difference between ground and first-excited states partially defines the "resolution" of the experimental data, and it is thus important to have the largest possible value of this quantity. Also the question of increasing the splitting between levels naturally arises when considering the DotFET concept.[21,22] Several groups have theoretically addressed the electronic structure of SiGe/Si islands with different structural parameters.[16,18,23–26] In the present work we calculate the energies of the lowest localized states of electrons in the Si matrix for two classes of experimentally relevant SiGe 3D islands with realistic structural parameters. On that basis, conditions for the robust confinement are revealed which provide the minimum ground-state energy and the maximum-energy splitting between the lowest energy states.

II. PROBLEM DEFINITION AND MODEL

We take for our modeling two different island shapes typically observed in the SiGe/Si(001) system:[27] a pyramid with {105} facets [inset of Fig. 1(a)] and a dome consisting of four {1 0 5}, four {1 1 3}, and eight {15 3 23} facets [inset of Fig. 1(b)]. Islands are usually made of an inhomogeneous SiGe alloy even when pure Ge is deposited on Si because of intermixing.[28] Alloying reduces the effective mismatch with the substrate, leading to an increase in the typical island size. We first assume the islands to be made of a homogeneous $Si_{1-x}Ge_x$ alloy. While this situation is poorly met by SiGe islands obtained by Ge deposition on flat substrates (see below), islands with rather homogeneous alloy compositions can also be realized by codeposition of Si and Ge (Ref. 23) or by growth of Ge on prepatterned substrates.[25,29,30] A latter approach is particularly relevant for the potential realization of single-dot-based devices. The linear sizes (width L and height H, see Fig. 1) scale with x according to (see, e.g., Ref. 31)

$$L(x) = L_0/x^2, \quad H(x) = H_0/x^2. \tag{1}$$

For the initial linear sizes of a pyramid (L_0^P, H_0^P) and a dome (L_0^D, H_0^D) we assume $L_0^P = L_0^D = 10$ nm, and $H_0^P = 1.41$ nm, $H_0^D = 4$ nm in accordance with available experimental data (see, e.g., Ref. 28). (We verified the accuracy of this assumption by comparing the sizes of islands with average Ge fraction x down to about 0.3). We assumed that the island shape and composition are preserved during encapsulation in Si,

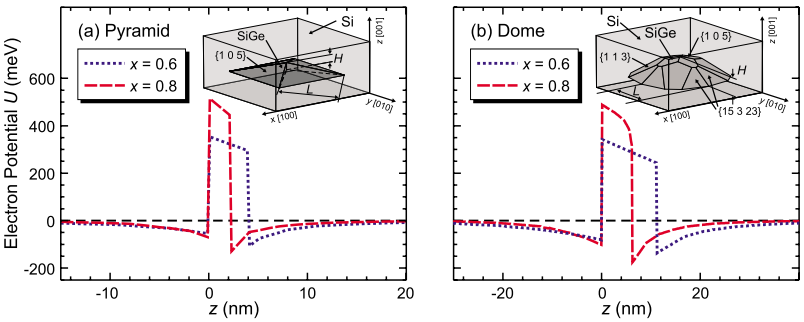

FIG. 1. (Color online) Conduction-band edge along the growth direction z through the center of (a) a pyramid and (b) a dome. Insets show the island geometries.

which can be experimentally realized by Si overgrowth at low substrate temperature.[32] The strain is calculated by the finite element method with the COMSOL MULTIPHYSICS software. Following the idea of the "model-solid theory,"[33] we determine the band lineup at the SiGe/Si interfaces taking into account the effects of composition and strain. The strain-induced potential is

$$U(\mathbf{r}) = E_{c,\mathrm{SiGe}}^{\mathrm{strain}}\chi(\mathbf{r}) + E_{c,\mathrm{Si}}^{\mathrm{strain}}[1-\chi(\mathbf{r})] - E_{c,\mathrm{Si}}^{0}, \qquad (2)$$

where $E_{c,\mathrm{Si}}^{0}$ is the energy reference level taken at the minimum of the Δ-valley conduction band of unstrained Si, $E_{c,\mathrm{SiGe(Si)}}^{\mathrm{strain}}$ is the energy conduction-band edge in strained material,[33] and $\chi(\mathbf{r})=1(0)$ when the position-vector $\mathbf{r}$ lies inside (outside) the SiGe island. Figure 1 shows the typical band alignment for two types of islands, a pyramid and a dome, for different values of x, which affects the island size according to Eq. (1). The potential height inside the island obviously decreases with decreasing x while it is not affected much by the island shape. The island shape (more precisely, the H/L ratio), produces, however, relevant differences in the potential in the Si matrix near the apex and the bottom of the island: the "dome-induced" potential well is deeper and broader than that for the pyramid. From Fig. 1 we see that electrons can be confined near the apex and the base of the island for both pyramids and domes, but the latter provide a stronger confinement. With decreasing x, the strain spread in Si becomes less pronounced. However, a simultaneous increase in island size partly compensates this effect so that a detailed calculation is needed to find the optimum conditions to achieve the deepest potentials.

To find the confined states of electrons we solve the Schrödinger equation using the effective-mass approximation

$$\left(\frac{\hat{p}_x^2+\hat{p}_y^2}{2m_{xy}} + \frac{\hat{p}_z^2}{2m_z}\right)\psi + U(\mathbf{r})\psi = E\psi, \qquad (3)$$

where $U(\mathbf{r})$ is defined by Eq. (2) and $\hat{p}_\xi^2 = -\hbar^2\frac{\partial^2}{\partial\xi^2}$, $\xi = x,y,z$. We take the values of the effective masses at the Δ minimum in Si as $m_z = 0.92m_0$ and $m_{xy} = 0.19m_0$,[34] where m_0 is the free-electron mass.

III. RESULTS AND DISCUSSION

Figure 2 shows the energy dependence of the lowest localized states on x (E_{s1}^{D} and E_{s1}^{P} are the energies of the ground states and E_{p}^{D} and E_{p}^{P} of the first excited states located near the apex of a dome D and a pyramid P while E_{s2}^{D} and E_{s2}^{P} are the energies of the lowest states located near the island bottom). We changed x in the range $0.3 \le x \le 0.8$. In the experiment, *average* compositions in this range can be obtained by simply varying the substrate temperature during Ge deposition. The minimum ground-state energy (~ -75 meV) is obtained for a dome with $x=0.7$, which has sizes $L=20$ nm and $H=8$ nm. At $x=0.7$, we note an accidental degeneracy of the states E_{s2}^{D} and E_{p}^{D} (~ -56 meV). Interestingly, the separation between E_{s1}^{D} and E_{s2}^{D} for a dome is practically constant (~ 20 meV) while the splitting between E_{s1}^{D} and E_{p}^{D} reaches a maximum of ~ 24 meV at $x=0.8$ and gradually decreases within decreasing x. For comparison, the difference between the two lowest levels for states localized on shallow donors is approximately 10 meV,[19] highlighting the potential advantage of using SiGe islands to confine electrons in Si.

The localized states of electrons for a pyramid show similar trends as for a dome but the absolute values of their energies are smaller. Values of both the ground-state energy and of the energy splitting $E_{s1}^{P}-E_{p}^{P}$ for a pyramid are comparable with those for donors. Hence a dome structure with a homogeneous composition in the range $0.6 < x < 0.8$ is preferable to a pyramid for electron-confinement purposes.

Below we study the influence of different growth regimes on the electron confinement. While islands with rather homo-

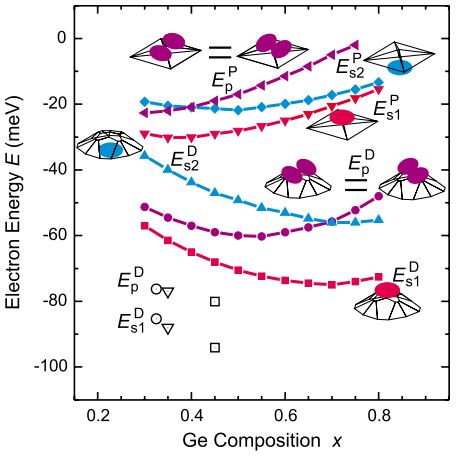

FIG. 2. (Color online) Energy of the lowest confined electron states as a function of Ge composition x in homogeneously alloyed islands. Insets show the island geometry and the electron-probability density distribution for the different states (isoprobability surface). The points correspond to cases of islands grown at a substrate temperature of 620 °C (□), 700 °C (▽), and 750 °C (○) and with compositional gradients taken from Ref. 35.

geneous composition distributions can be experimentally obtained under certain growth conditions,[23,25,29,30] islands obtained by deposition of only Ge on planar substrates usually have a Ge-rich top and a Si-rich base.[28,35,36] To have an idea of the effect of a composition gradient in the growth direction, we have calculated the confined states for domes grown at substrate temperatures T of 620, 700, and 750 °C and using the composition profiles reported in Ref. 35. The results for E_{s1}^{D} and E_{p}^{D} are shown with symbols in Fig. 2 as a function of the estimated average Ge content. The data indicate that vertical gradients in the Ge content give rise to a significant strengthening of confinement and a consequent shift of the energy of the localized states. Specifically, the comparison between islands having a Ge-rich top with islands possessing homogeneous composition but same average x shows that for the former $E_{s1}^{D}(E_{p}^{D})$ are on average 30(20) meV lower than for the latter. Both the lowering of the ground-state energy and the increase in energy separation between the first two levels are due to the Ge enrichment of the island apex, which produces a more pronounced strain compared to islands with a homogeneous composition.

Until now we have considered the situation in which the island shape is preserved during capping. Under usual conditions (Si capping performed at temperatures close to the Ge growth temperature), the shape of the islands changes. In a first approximation, Si overgrowth leads to material redistribution involving the removal of the apex of the islands. (Ge-rich material moving away from the island top intermixes with Si and is redeposited at the island sides).[36] This phenomenon leads to substantial changes in the confinement energy especially for islands with an initially pronounced vertical x gradient, as illustrated in Fig. 3, where we compare calculations for a homogeneously alloyed island (with $x=0.47$) and for an island with a strongly inhomogeneous composition, taken from the experiments of Ref. 36. For the realistic structure (with average Ge fraction of 0.47) and assuming shape preservation during capping ($\alpha=1$, see caption of Fig. 3) the energies E_{s1}^{D} and E_{p}^{D} are ~120 meV and ~100 meV below the reference level, respectively. The corresponding values for the homogeneously alloyed island are 69 and 59 meV. The progressive cutoff of the island top leads to an increase in the ground-state energy and a reduction in the energy splitting between the ground state and the first excited state.

IV. CONCLUSIONS

In summary, we have investigated the effect of SiGe island morphology and composition on electron confinement in the surrounding Si matrix. For the case of homogeneously alloyed islands, domes with Ge content in the range $0.6<x<0.8$ provide the best electron confinement. The ground-state energy and the energy splitting between levels for such islands are more than two times larger than those for pyramid structures. We have evaluated the effect of the composition distributions and the shape change due to the growth conditions on the electron confinement. For structures with realistic Ge distributions characterized by a Ge fraction increasing from the island base to the apex, confined levels as deep as ~120 meV below the continuum may be achieved provided that the island structure is preserved during the Si overgrowth. However, capping at high substrate temperatures appears deleterious, as the removal of the Ge-rich top produces a substantial reduction in electron confinement. This work guides the design of SiGe/Si structures providing robust electron localization in Si for experimental studies on electron spins[17] localized in Si/SiGe QDs. Field-effect transistors based on single SiGe/Si dots[37] will allow for addressing single-electron spins.

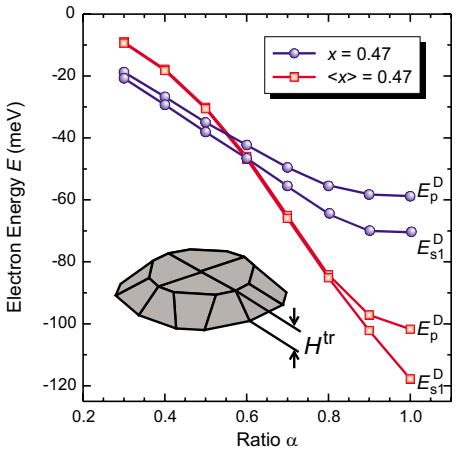

FIG. 3. (Color online) Modeling of the effect Si capping at high substrate temperature on the energies E_{s1}^{D} and E_{p}^{D}. The capping produces a truncation of the dome and consequent height reduction from H to H^{tr} (see inset). $\alpha=H^{tr}/H$. Circles correspond to a homogeneously alloyed island and squares correspond to the inhomogeneous composition from Ref. 36.

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*r.rezaev@ifw-dresden.de

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