Pair interaction between Ge islands on vicinal Si(001) surfaces

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The pair interaction between Ge islands on vicinal Si(001) substrates is investigated by scanning tunneling microscopy measurements as a function of the miscut angle. By the analysis of the nearest-neighbor island distributions, we assess the dependence of the local strain field on the substrate misorientation. We support our results by modeling elastic relaxation for different shapes and arrangements of islands with finite element calculations.

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Miniaturizing electronics with the ultimate goal of developing tomorrow's functional devices has been pushing the lithography techniques down to the nanometer-scale breaking point where they face major intrinsic limitations. At present, the most challenging task in nanoscale science is the formation of ordered nanostructures by self-organization.[1–5] This amounts to taking advantage of the Stranski-Krastanov epitaxy of lattice-mismatched semiconductor materials to obtain self-assembled nanoislands. In order to make the transition from basic physics to technology, some control over island position is required. To this purpose, a detailed comprehension of island's interaction is needed. A possible approach is to study first the interaction between nearest-neighbor islands. As a model system, we chose Ge on vicinal Si(001), which allows us to tune both the energetic and the kinetic factors governing the growth of single nanostructures by changing the substrate miscut. In fact, the local ordering may depend either on the mass transport among islands, or on the strain field which governs elastic interactions between them.[6,7] On vicinal Si(001) surfaces, both the anisotropy in surface migration[8] and the island shape (i.e., the strain field profile inside and around each island) (Ref. 9) are strongly dependent on the miscut angle, thus permitting an accurate evaluation of both. From a systematic scanning tunneling microscopy (STM) study of the spatial distribution of nearest-neighbor Ge islands as a function of the substrate vicinality, we gather information on the elastic interaction among self-organized nanostructures.

Experiments were carried out in ultrahigh-vacuum chamber ($p<3\times10^{-11}$ torr). We used Si(001) wafers with azimuthal angle $\phi=0°$ and polar miscut angle θ ranging between 0° and 8° toward the [110] direction. The substrates were cleaned *in situ* by a standard flashing procedure at 1473 K. The Ge was deposited by physical-vapor deposition at 873 K under a constant flux of $(5.3\pm0.6)\times10^{-2}$ ML/s. The flux was calibrated from the increasing area of terraces between two successive STM images during the layer-by-layer growth.[10] STM measurements were carried out at room temperature in the constant-current mode, using W-probe tips.

Figure 1 shows the morphological evolution of Ge islands on vicinal Si(001) substrates as a function of miscut angle. Islands elongate in the miscut direction as the substrate vicinality is increased,[11] finally forming wirelike ripples at 8° miscut angle.[12] The spatial organization of islands depends both on surface diffusion and on the interaction among the elastic strain fields linked to each island. Moreover, the detailed island shape, which depends on miscut angle, crucially determines the local elastic field. The diffusion field is also affected by substrate vicinality: the flat Si(001) surface consists of alternating (1×2) and (2×1) domains. On these domains, the fast diffusion directions are different and orthogonal to each other;[13] when the miscut angle is increased, the (1×2) domains gradually disappear and an evolution to a surface mostly (2×1) reconstructed takes place.[14] On the mesoscale, this means that, when the miscut is high enough, the diffusion tends to be anisotropic along the (2×1)-fast diffusion direction, namely, the [110] direction. In order to study the local spatial ordering of islands, we have measured the spatial distribution of nearest-neighbor distances (SDNN) on different miscut substrates. First the centers of mass of all islands are identified. Then, for each island, the nearest-neighbor island is found by calculating the distances between the corresponding centers of mass.[15] Each panel in Fig. 2 shows the position of the nearest neighbors measured on the related vicinal substrate. The color scale represents the relative density of nearest neighbors. It can be seen that SDNN is almost isotropic for flat substrates, whereas, increasing the miscut angle, the higher density of nearest neighbors along the [110] direction signals that the local arrangement of the islands becomes anisotropic.

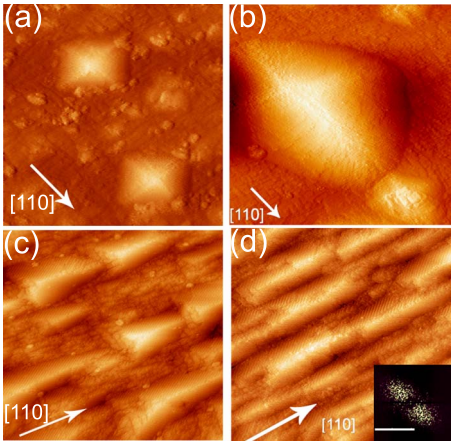

FIG. 1. (Color online) STM images of Ge islands on Si(001) at (3.2 ± 0.4) ML of coverage: (a) $(100\times100$ nm$^2)$ flat, (b) $(150\times150$ nm$^2)$ 1.5°-miscut, (c) $(120\times120$ nm$^2)$ 6°-miscut, and (d) $(100\times100$ nm$^2)$ 8°-miscut surfaces. The inset shows the FFT transform of the 8° image. The scale bar length is 0.05 nm^{-1}.

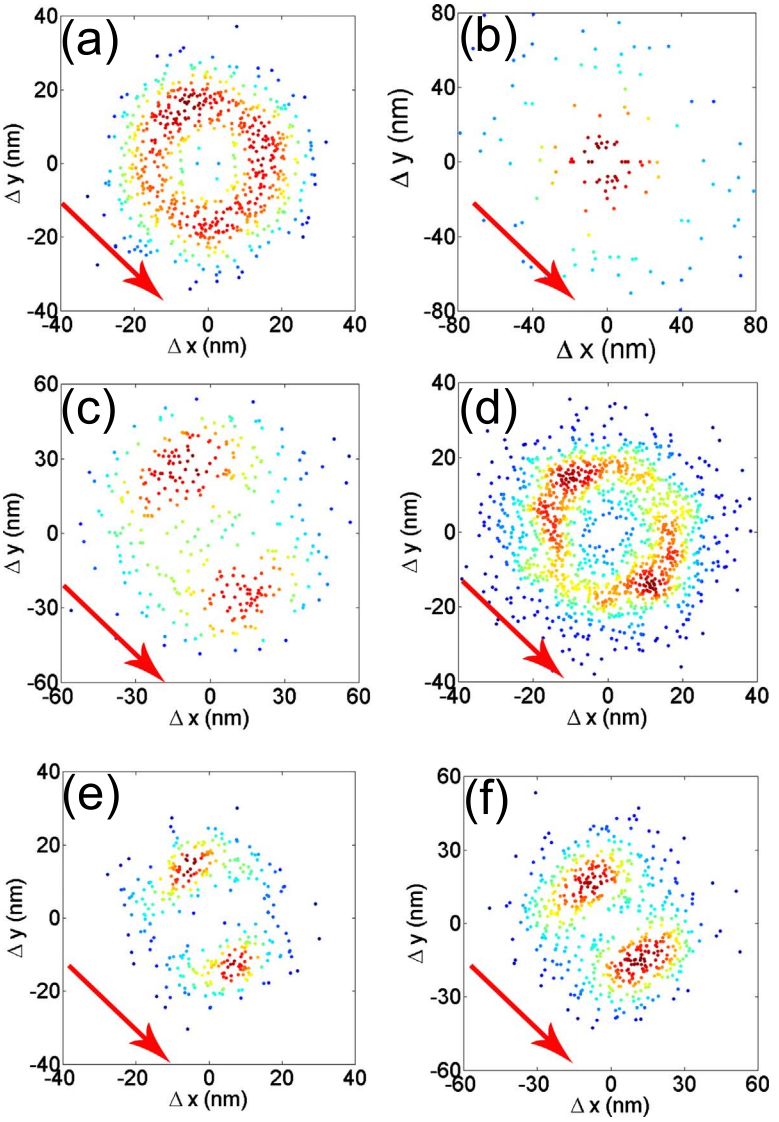

FIG. 2. (Color online) Spatial distribution of nearest-neighbor distances of Ge islands on: (a) flat, (b) 1.5°-miscut, (c) 2°-miscut, (d) 4°-miscut, (e) 6°-miscut, and (f) 8°-miscut Si(001) samples. The arrows indicate the [110] direction.

Hence, the analysis of STM images indicates that the miscut angle modifies the local spatial organization of Ge islands. This is likely to be associated with the anisotropy of the diffusion coefficient, which increases the local density of adatoms along the miscut direction, and then the island nucleation. Besides, the elastic pair interaction between islands is also strongly affected by the misorientation angle. Figures 3(a)–3(c) shows finite-element calculations of the elastic interaction energy for all the Ge island shapes experimentally imaged on vicinal Si(001) substrates;[16] in each case we consider the two relevant configurations for an island pair. The interaction energy is evaluated as the difference between the elastic energy of the system (substrate+island pair) for islands separated by a distance d and for infinite separation. The elastic interaction between misfit islands was previously studied by modeling the associated forces as point force dipoles.[17] This approach is hence valid only at large distances, where the actual shape of the island is immaterial, and suggests that interaction energy varies as d^{-3}. On the basis of our analysis, which fully takes into account realistic three-dimensional island shapes, we find that on the flat surface the elastic interaction energy scales as d^{-3} at large distances, but it deviates from the point-island approximation at smaller separations. From Fig. 3(a), we note that on the flat surface the interaction energy is isotropic. On vicinal substrates, the detailed island shape cannot be neglected, because it introduces a strong directional dependence of elastic interactions. When the misorientation angle is increased, the lowest-energy configuration is achieved by aligning the pair along the miscut direction [Figs. 3(b) and 3(c)]. This is mainly due to the larger relaxation of the substrate in between the two islands, as shown by the energy maps at 6° and 8° miscuts [Figs. 3(d) and 3(e)]. In particular, when the density is increased, individual ripples on the 8°-miscut surface tend to coalesce along the [110] direction, forming the elongated ribbons shown in Fig. 1(d). This process results in a periodicity in the orthogonal direction, as evidenced by the fast-Fourier transform (FFT) of the STM image, reported in the inset.

In conclusion, we have demonstrated by a detailed STM study of Ge on several vicinal Si(001) surfaces that both the local strain and diffusion fields, which are responsible for short-range ordering, can be markedly affected by the miscut angle. The elastic pair interaction energy has been computed

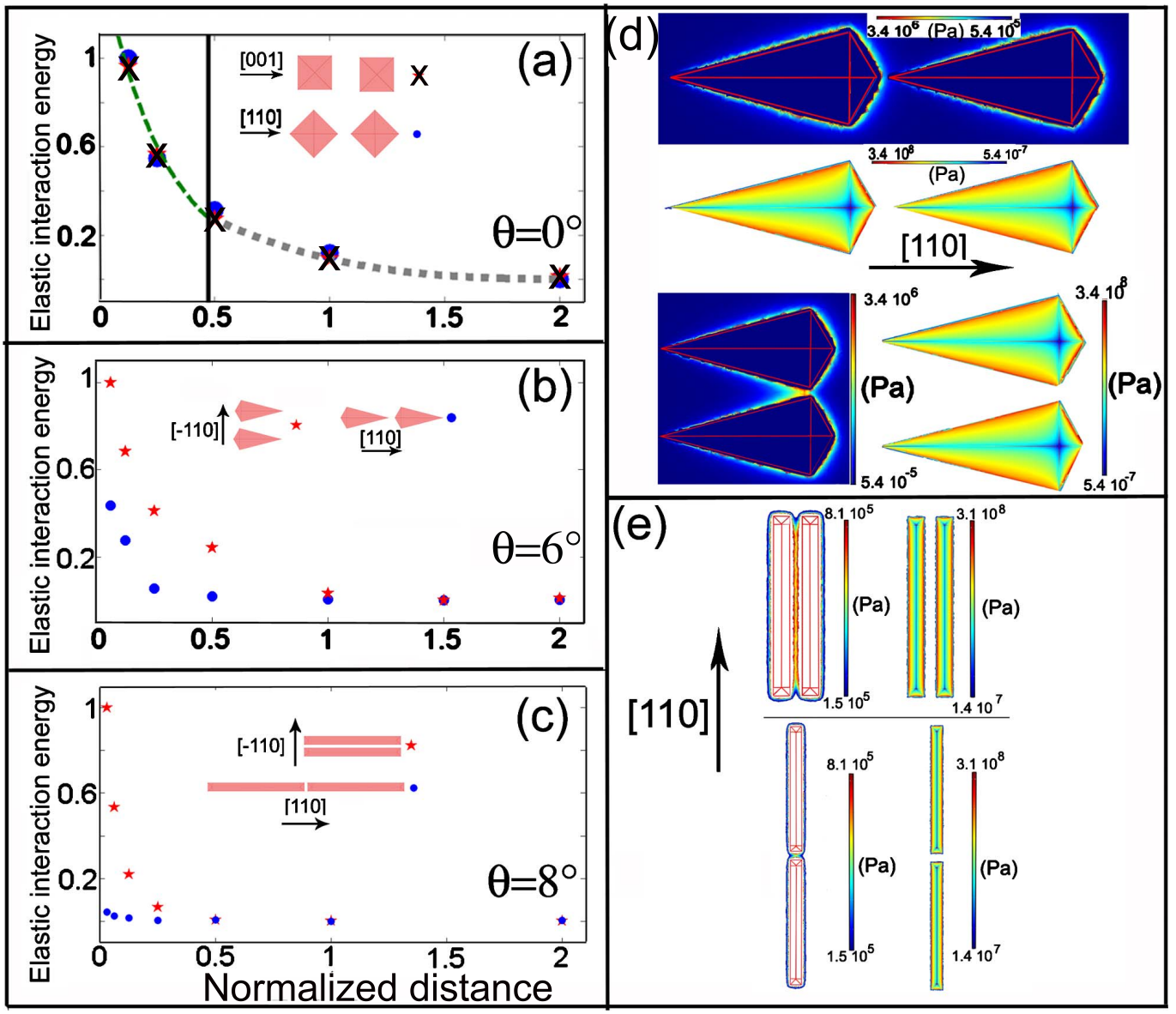

FIG. 3. (Color online) Finite-element method calculations of the elastic strain relaxation. Elastic interaction energy for different configurations of an island pair on (a) flat, (b) 6°-miscut, and (c) 8°-miscut Si(001) surfaces (vertical axis in arbitrary units, horizontal axis in units of the average island side). The data in the panel (a) are fitted to a d^{-3} function at large island separations (dot curve) and to an exponential function at short separations (dashed curve). The vertical line marks the boundary between the two regimes. Elastic energy density maps of an island pair on (d) 6°-miscut and (e) 8°-miscut surfaces. Each plot is displayed with two different scales giving the elastic relaxation within the islands and on the substrate around them.

for the realistic Ge island shapes grown on vicinal Si(001) surfaces, thus contributing to a better understanding of in-plane interactions among these nanostructures.

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