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Published in:
Physical Review Letters

Link to article, DOI:
10.1103/PhysRevLett.78.503

Publication date:
1997

Document Version
Publisher's PDF, also known as Version of record

Citation (APA):
Shiryaev, S. Y., Jensen, F., Hansen, J. L., Petersen, J. W., & Larsen, A. N. (1997). Nanoscale Structuring by Misfit Dislocations in Si1-xGex/Si Epitaxial Systems. *Physical Review Letters*, *78*(3), 503-506. https://doi.org/10.1103/PhysRevLett.78.503

Nanoscale Structuring by Misfit Dislocations in $Si_{1-x}Ge_x/Si$ Epitaxial Systems

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(Received 22 March 1996)

New capabilities of misfit dislocations for spatial manipulation of islands in $Si_{1-x}Ge_x/Si$ heteroepitaxial systems have been elucidated. Formation of highly ordered Ge-island patterns on substrates prestructured by slip bands of misfit dislocations is revealed. The major sources leading to the ordering are identified to be dislocation strain fields at the surface and modifications of the near-surface-layer morphology induced by dislocation slip. [S0031-9007(96)01997-7]

PACS numbers: 68.55.–a, 61.16.Bg, 61.16.Ch, 61.72.Lk

The interplay between surface morphology and misfit dislocations in heteroepitaxial semiconductor systems has recently been a subject of numerous studies [1]. It manifests itself in a diverse range of phenomena, such as formation of gradual surface undulations (cross-hatch patterns) arising from the surface mass transport driven by the strain fields of the misfit dislocations [2–4], elastic [5] and plastic [6] displacements of the surface by misfit dislocations, and dislocation nucleation at surface-ripple structures in continuous heteroepitaxial layers [7–10]. Alignment of the surface-ripple domains along dislocation lines was observed in $Si_{1-x}Ge_x/Si$ heteroepitaxial systems and attributed to ripple-dislocation interactions mediated by strain [7,10]. An ordering of InP islands on a strained InGaP buffer was found in Ref. [11] and explained by a preferential island nucleation driven by the misfit-dislocation strain. In this Letter we report on a new phenomenon—formation of highly ordered patterns of isolated Ge islands on $Si/Si_{1-x}Ge_x/Si$ substrates prestructured by the introduction of misfit dislocations. An outstanding feature of these patterns is that they are almost entirely composed of well-separated rows of sharply aligned Ge islands and mimic the underlying dislocation-slip-band morphology.

The basic idea of our experiments is illustrated in Fig. 1. A heteroepitaxial system is grown consisting of a compositionally graded $Si_{1-x}Ge_x$ layer on a (001) Si substrate and—on top of that—a uniform $Si_{1-x}Ge_x$ layer comprising a quantum well (QW) used as a marker layer, and finally a silicon cap layer. The structure is metastable and has been shown to relax during postgrowth annealing through a self-organized process leading to the formation of very narrow, shear bands of misfit dislocations in the graded layer [12]. This has dramatic consequences for the initial structure, such as the following: (i) formation of shear steps both on the surface and at the heterointerfaces in the bulk of the epitaxial system and (ii) appearance of a surface, elastic-strain pattern associated with the highly nonuniform distribution of the misfit dislocations in the graded layer. After relaxation, Ge is deposited on the surface to study the effect of the surface morphology and surface strain on the growth of three-dimensional (3D) Ge islands on Si.

The samples were grown at 530 °C by molecular-beam epitaxy (MBE) and included graded layers identical to those used in our previous work [13]. The top uniform $Si_{0.8}Ge_{0.2}$ layer included a 5 nm thick, $Si_{0.6}Ge_{0.4}$ QW and a 10 nm thick Si cap. The relaxation of the mismatch strain in the samples was achieved directly in the MBE chamber by flashing the substrate temperature up to 800 °C for 15 s. After the flash the temperature was reduced to 740 °C and a Ge film with a nominal thickness of 1.2 nm was deposited on top of the relaxed structure, at a deposition rate of 0.02 nm/s. For comparison, the same amount of Ge was also deposited on the surface of a virgin Si substrate and on the surface of the above heterostructure without a Si cap.

The atomic force microscopy (AFM) images displayed in Fig. 2 illustrate the results of the Ge deposition on the surface of a virgin (001)Si wafer (a) and of prestructured $Si_{1-x}Ge_x/Si$ (b) and Si-cap/$Si_{1-x}Ge_x/Si$ substrates (c). Well-defined Ge islands are resolved in all the images indicating 3D growth in all the cases. The islands are randomly distributed on the surface of the Si substrate [Fig. 2(a)] in agreement with previous observations of Ge islanding on (001) Si (see, for example, Ref. [14]). In contrast to this structure, ordered Ge-island patterns are

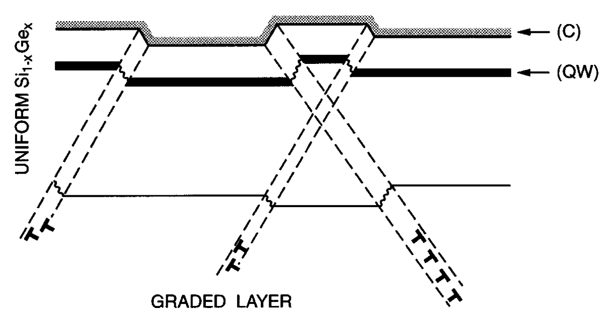

FIG. 1. Schematic diagram illustrating the structuring of $Si/Si_{1-x}Ge_x/Si$ substrate with dislocations in a compositionally graded layer. The dashed lines illustrate the regions of dislocation slip. C and QW denote a Si cap and a quantum well, respectively.

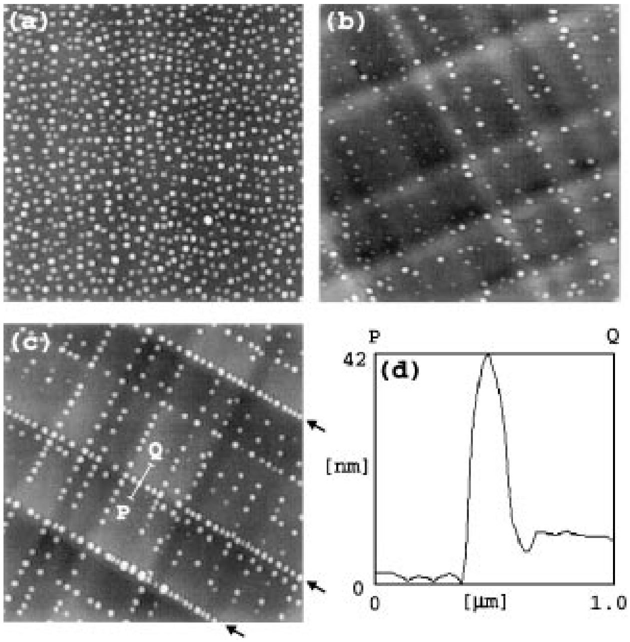

FIG. 2. AFM image of a 7.7 × 7.7 μm^2 surface area showing the result of deposition of a 1.2 nm thick Ge film on the surface of a bare (001) Si substrate (a) and patterned $Si_{1-x}Ge_x/Si$ (b) and $Si/Si_{1-x}Ge_x/Si$ (c) systems. The height scale (black to white) is (a) 41 nm, (b) 53 nm band, and (c) 63 nm, respectively. A height profile (d) through an island in (c) along the line P-Q is shown.

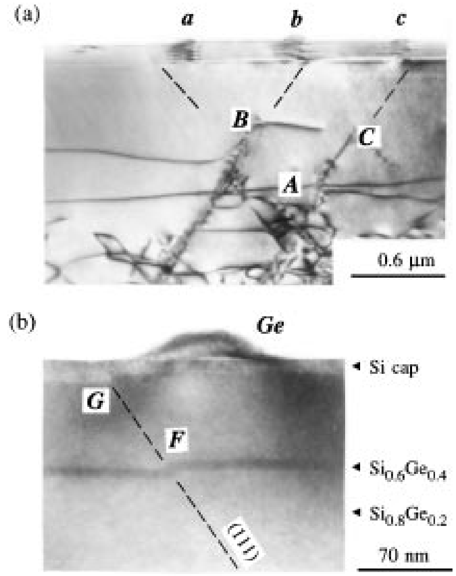

FIG. 3. Cross-sectional TEM images of the sample shown in Fig. 2(c). (a) Rows (a, b, and c) of Ge islands are aligned along the [110] surface direction. The sample is tilted off the [110] zone axis to visualize the (001) surface thereby displaying the rows of Ge islands. (b) Enlarged TEM image of one island (F and G mark the steps produced by a shear band on, respectively, the $Si_{0.6}Ge_{0.4}$ marker, and the interface between the Si cap and $Si_{0.8}Ge_{0.2}$). The dashed lines indicate {111} slip planes corresponding to particular bands in the graded layer.

found on the surfaces modified by the misfit dislocations [Figs. 2(b) and 2(c)]. The islands formed on the surface of bare $Si_{0.8}Ge_{0.2}$ [Fig. 2(b)] are distributed dominantly in relatively wide straps oriented along ⟨110⟩ surface directions. Although a weak geometrical correlation can be seen on this surface (a part of the islands accumulates around the transition regions between elevated and depressed areas of the surface), the islands do not preferentially populate the depressions or elevations.

A spectacular effect is observed on the surface of the heterostructure with the Si cap. The island pattern found in this case [Fig. 2(c)] mimics the slip morphology of the surface and almost all (about 90%) Ge islands are aligned in sharp rows parallel to the ⟨110⟩ surface directions. Height profiles through the islands [see Fig. 2(d)] reveal that the islands are located at the edges of the shear steps. Furthermore, in case (a) the fraction of the surface area covered with the islands (18%) is much higher than that in case (c) (8%). Note also that the island rows in case (c) are separated by large rectangular areas completely free of islands. These observations suggest that Ge from these areas redistributes to the islands in the rows [15] leaving the Ge-film thickness in these areas in the range of the wetting-layer thickness (≈3 ML [16]).

The spatial relationship between the Ge islands and the misfit dislocations in the sample shown in Fig. 2(c) becomes apparent in cross-sectional TEM images (Fig. 3). The Ge islands are now seen to be localized in the vicinity of the slip regions on the surface (the so called band-yield regions). In Fig. 3(a) island rows a, b, and c propagate along the [110]-surface directions perpendicular to the cross-sectional plane and are positioned at the yield regions of, respectively, bands A, B, and C composed of dislocations gliding on the (111) (A) and $(1\bar{1}1)$ (B and C) planes perpendicular to the cross-sectional plane.

Figure 3(b) is a magnified image of one island and the underlying structure. The yield region of the slip band corresponding to this island is defined in Fig. 3(b) by the (111) plane intersecting slip step F on the $Si_{0.6}Ge_{0.4}$ marker and slip step G at the interface between the Si cap and the underlying $Si_{0.8}Ge_{0.2}$ layer. It can be recognized that the position of the Ge island is displaced from the band-yield region to the elevated part of the step structure. Detailed examination of cross-sectional images shows that this spatial relationship is characteristic of islands aligned along the band-yield regions. This observation is consistent with the AFM images where such a relationship is found for a number of Ge rows [marked by arrows in Fig. 2(c)]. On the other hand, inspection of the cross-sectional images of the noncapped samples revealed no such spatial correlation between the islands and slip-band regions; the islands in the straps were found at both sides of these regions. In addition, a heavy strain contrast was found in both the islands and the substrate just below the islands for all the samples shown in Fig. 2. Hence, we conclude that they belong to the category of islands which are partially relaxed through elastic displacements in both the island and the substrate [14].

A characteristic feature of the capped samples is that the Si-cap thickness is locally decreased at the elevated sides of the bulk slip steps [*G* in Fig. 3(b)] and locally increased at the opposite sides. In the areas remote from the band-yield regions this thickness reaches its nominal value of 10 nm. We found that this modification of the Si-cap layer occurs during annealing in the MBE chamber before the Ge deposition, and attribute this effect to a surface redistribution of Si which results in a smoothing of the sharp slip-step bunches highly energetically unfavorable on the free surface.

In general, there are several sources which may provide energetically favorable sites for island location on the surface. They include surface steps [17,18], local deviations of the surface from planar orientation [19], and the nonuniform strain at the surface which provides the sites with a reduced mismatch between Ge and Si [10,20,21]. The island positions found in our case do not coincide with the slip steps on the surface either for noncapped or capped samples. Therefore, we conclude that the island ordering observed in the present work is not mediated by the slip steps. Furthermore, the islands in the noncapped samples do not preferentially populate the elevations or depressions on the surface. Hence, the only source which can induce the highly nonuniform island distribution in this case is the nonuniform elastic strain from the dislocation bands. This conclusion is supported by the results of recent experimental and theoretical studies of the vertical self-alignment of islands in multilayered heteroepitaxial systems [20,21] and alignment of InP islands on strained InGaP buffers along dislocation bunches [11]. Although these studies focus on the different aspects of the island formation process (either island-nucleation events [20] or surface diffusion leading to a nonuniform thickness of the wetting layer [21]), they imply a common driving force for the island alignment which is nonuniform strain at the surface.

The above results show that the presence of the Si cap has a dramatic influence on the island pattern which manifests itself in the extremely sharp island alignment along the band-yield regions. There is also a significant difference in the island-size distributions for the capped and noncapped samples [see Figs. 2(b) and 2(c)]. In this work we focus on the most striking effect which is the sharp alignment. To explain this effect we shall consider the near-surface layer structure which includes the Si cap and the interface between the cap and the $Si_{0.8}Ge_{0.2}$ layer. There are two features of this structure that may contribute to such an alignment. The first feature is the sharp steps at the interface between the tensile-strained Si cap and the relaxed $Si_{0.8}Ge_{0.2}$ layer [*G* in Fig. 3(b)]. Because these slip steps perturb the biaxial strain between the Si cap and $Si_{0.8}Ge_{0.2}$, and lie very close to the surface, they induce local surface-strain variations and, thus, may provide low-energy sites for the islands. The second feature is the local variation in the Si cap thickness around the band-yield regions. It appears that the positions of the islands correspond to those sides of the regions where the thickness of the Si cap film is smaller [Fig. 3(b)]. This correlation suggests that the substrate sites with a thinner Si cap may be energetically more favorable for the islands than the sites with a thicker Si cap. A reason for this may be that the substrate in these regions is "softer," i.e., it allows larger elastic deflections of the Ge/Si interface from the planar orientation providing a higher degree of the elastic relaxation in the islands. This suggestion is based on recent calculations which show that the elastic displacement fields originating from islands penetrate to substrate depths larger than the island heights [22]. Therefore, since the Si cap thickness in our case is smaller than the island heights, both the Si cap and underlying $Si_{0.8}Ge_{0.2}$ alloy volumes are involved in the relaxation. Note that the substrate regions under the islands where the cap is thinner include smaller Si volumes per unit surface area. Hence, these regions are softer because Si has larger elastic constants than $Si_{0.8}Ge_{0.2}$ [23]. Finally, the present results do not allow for a decoupling of the effects of the near-surface steps and the Si-cap thickness. Thus we cannot make any clear conclusions concerning their relative role in the sharp island confinement. A separation of these effects would, however, be of great interest not only from a scientific but also a technological point of view since it may provide new routes for the alignment of nanodot structures.

In summary, new capabilities of misfit dislocations for spatial structuring of heteroepitaxial semiconductor systems at the nanometer length scale have been elucidated. Formation of ordered Ge-island patterns on $Si_{1-x}Ge_x/Si$ and Si-cap/$Si_{1-x}Ge_x/Si$ substrates prestructured by dislocation bands is revealed. The most spectacular ordering was observed on surfaces of samples with Si caps where the islands appear to be confined to one-dimensional rows aligned along slip regions on the surface. It was demonstrated that the ordering of the islands is not mediated by the slip-step bunches on the surface. The results suggest that the ordering on the noncapped substrates originates from the nonuniform dislocation strain fields and that the sharp lateral confinement of the islands on the capped substrates is mediated by the near-surface layer structure modified by the dislocation slip. Although the analysis done in this work is qualitative and omits aspects of island nucleation and growth [8,18,24], it captures, in our opinion, the major sources which may lead to the sharp lateral island confinement, and thus provides a framework for further, detailed studies.

This work was supported by the Danish Minister of Industry and Research in the framework of CNAST. Special thanks to Pia Bomholt for the help in the preparation of the cross-sectional TEM specimens.

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