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Computation of the preferential nucleation sites for Ge quantum dots on a relaxed SiGe layer

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Abstract

We compared directly the nucleation sites of Ge quantum dots on a relaxed SiGe buffer layer with the sites of a minimum stored energy density of the Ge dots. The computed elastic stored energy of the Ge dots encompasses the effect of both lattice mismatch and misfit dislocations. We computed the strain/stress of the misfit dislocations near a free surface by using the solution presented by Gosling and Willis [J Mech Phys Solids 1994;42:1199]. The study revealed that the intersection of the slip-planes with the free surface is the site of the maximum tensile strain, thus the Ge dots, which have a negative misfit, preferentially nucleate at that site. Our work clearly demonstrates the role of misfit dislocations in the formation of the ordered array of Ge dots. We also discuss the application of misfit dislocations for selective etching and the effects of a free surface on the displacements of the underlying misfit dislocations.

Keywords: Atomic force microscopy; Dislocation theory; Quantum dots; Thin films

1. Introduction

We computed the stress field originating from misfit dislocations in the SiGe/Si system in order to explain the role of misfit dislocations in forming spatially ordered quantum dots (QDs). Numerous experiments have shown that a misfit dislocation acts as an inducer for the ordered spatial distribution of QDs and that the location of the QDs is offset to one side of the dislocation. We found the origin of the spatially biased nucleation of the QDs. We compared the computed nucleation sites of the QDs with the experimentally observed sites using a transmission electron microscope (TEM).

Excessive lattice mismatch during a heteroepitaxial growth can lead to the formation of QDs under specific conditions. The growth mode of these three-dimensional (3D) dots, i.e. Volmer–Weber (island growth) and Stranski–Krastanow (layer-by-layer plus islands) mode, was proposed long before the actual experimental observation was made [1]. Because 3D dots often form spontaneously by partially relaxing the elastic strain energy due to a lattice mismatch, they are often called self-assembled quantum dots (SAQDs). Since the InAs/GaAs systems first showed such SAQD formations [2], various other systems have shown the formation of SAQDs, e.g. Ge/Si (IV systems), InGaAs/GaAs (III–V systems) and CdTe/ZnTe (II–VI systems). SAQDs usually form randomly in a space, but surprisingly they are uniform in size and shape [3]. It is, however, desirable to control the spatial distribution of SAQDs in order to be able to use the dots in device applications.

Regular in-plane spatial distribution could be achieved: (i) InAs dots buried in GaAs layers lead to vertically self-organized dots [4]; (ii) surface steps, which are formed artificially on an Si substrate, provide preferential positions for Ge dots [5]; and (iii) misfit dislocations affect the elastic state of the surface, which leads to an organized spatial distribution of the QDs [6,7]. Recently, focused ion beam (FIB) pre-patterning of Si substrates guided the positioning

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of the dots with a precision of tens of nanometers [8]. Properties of these organized SAQDs could open up various applications for new types of devices. Optical properties of QDs could lead to the development of lasers with high gain and low threshold currents [9] and their electronic properties could substitute for transistors in well-assembled QDs in a logic-function implementation [10].

Among the various inducers for ordered QDs, this paper is concerned with misfit dislocations located at the interface of an SiGe buffer layer and an Si substrate. Experimental observations [6,7] have shown the correlation between QDs and buried misfit dislocations in SiGe/Si epitaxial systems. More specifically, the dots form at the intersections of the slip-planes of a corresponding dislocation and the top surface in the SiGe/Si system [11,12], thus the preferential location of the QDs is offset to one side of the dislocation. The origin of this result is controversial; misfit dislocation may form steps (terrace) at an atomic scale on the top surface of SiGe or a heterogeneous strain field due to a misfit dislocation may provide preferential locations.

To verify the role of misfit dislocations in controlling the nucleation sites of QDs, the elastic stress/strain field of misfit dislocations was computed [14,15]. In these studies, a periodic array of dislocations represented the misfit dislocations at the interface of a buffer layer and a substrate, and the dislocations were of pure edge or screw type. Thus the configuration of misfit dislocations is simplified for the sake of a computational simplicity. The computation showed that misfit dislocations modulate the strain field of the top surface and provide low mismatch sites, i.e. preferential nucleation sites of the QDs. However, a precise computation that demonstrates how the preferential sites are the intersections of the slip-planes and the top surface in the SiGe/Si system has not hitherto been made. Direct comparison between computed sites and experimentally observed ones is still unavailable.

In real systems, misfit dislocations are often of the $1/2\langle 1\,1\,0\rangle$ Burgers vector type [16] and they show a non-periodic spatial distribution. For a computation, it is desirable to construct the same spatial array of misfit dislocations as observed in real systems in order to demonstrate the role of the misfit dislocations precisely. The main hurdle in this computation is the solution of the three-dimensional stress field due to a misfit dislocation array with arbitrary Burgers vectors and an arbitrary spatial distribution near a free surface. This problem is equivalent to computing the image stresses [17] of arbitrary misfit dislocations. The dislocation community has widely developed the methods for computing image stresses (see [18] and references therein), since there are numerous situations where dislocations are affected by image stresses, e.g. dislocations near voids, second-phase particles and microcracks. The developed methods were also applied to the problem involving thin films [19] and the effects of image stresses on the behavior of underlying dislocations were of concern in this work. It is generally agreed that the image effects are relatively small in simulations of a layer relaxation. However, the effect of underlying dislocations on the free surface can be very significant and it will be shown here that even the sign of the stress state can be changed due to the free surface effect. The formation of ordered QDs is also a dislocation problem for which image stresses are very important.

In this paper, we adopt the solution of Gosling and Willis [20] for computing the stress fields of misfit dislocations near a free surface. The work of Gosling and Willis provides an analytical solution of the stresses due to an arbitrary dislocation in an isotropic half-space. We show that the strain field of the top surface modulated by a misfit dislocation determines the position of the QDs on the misfit dislocation. We compare the computed preferential sites of the QDs with the experimentally observed ones by taking the same Burgers vectors and line directions for the computation as those determined by TEM.

2. Computation methodology

A volume of the computation comprises the free surface of a buffer layer which lies at $z = 0$, i.e. perpendicular to the $(0\,0\,1)$ axis. The x and y axes follow the directions of the $(1\,0\,0)$ and $(0\,1\,0)$ crystal axes, respectively. Misfit dislocations, which accommodate the misfit between a buffer layer and a substrate, are assumed to follow two $\langle 1\,1\,0\rangle$ directions at $z = d$ (thickness of the buffer layer). This configuration is equivalent to that of the experimentally observed misfit dislocations in a SiGe buffer layer on an Si $(0\,0\,1)$ substrate.

The formation energy, $w(x,y)$, of a QD at position x, y, $z = 0$ can be expressed as the sum of the surface energy, the local elastic stored energy of a QD and the interfacial energy between a QD and a buffer layer. If we assume that the surface energy and the interfacial energy are spatially constant, the local elastic stored energy is the only spatially variable term and $w(x,y)$ of a QD is expressed as the local elastic stored energy per unit volume of a QD [14]:

$$w(x,y) = \frac{1}{2}\sum_{i,j}(\sigma_{ij}^{m} + \sigma_{ij}^{d})(\varepsilon_{ij}^{m} + \varepsilon_{ij}^{d}). \tag{1}$$

σ_{ij}^{m}, ε_{ij}^{m} are the stress and strain experienced by a coherent QD due to the misfit, f_0, defined as $(a_{\text{layer}}^{0} - a_{\text{QD}})/a_{\text{QD}}$ with respect to the non-deformed buffer layer. The terms a_{layer}^{0} and a_{QD} are a lattice constant of the non-deformed buffer layer and a QD, respectively. The terms σ_{ij}^{d} and ε_{ij}^{d} are, respectively, the stress and strain experienced by the free surface of the buffer layer due to the misfit dislocations at $z = h$.

In Eq. (1), we did not consider the relaxation of a QD, thus a QD is elastically deformed to be epitaxially accommodated on a buffer layer. In reality, a QD and a buffer layer are elastically relaxed after adhesion, because normal stress components of the free surfaces of a QD vanish. This relaxation leads to a decrease in the total elastic energy and $w(x,y)$ of a QD decreases, whereas the elastic energy of a