MULTISCALE MODEL FOR GERMANIUM QUANTUM DOTS IN SEMI-INFINITE SILICON

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ABSTRACT

We have developed a multiscale model for quantum dots in semiconductors that links the length scales from sub-nano to macro. The model is computationally efficient and can be used on an ordinary desktop computer even for a crystallite containing a million atoms. It is necessary to model a large crystallite for large quantum dots to avoid spurious size effects. The model integrates the classical molecular dynamics with Green's functions. We use molecular dynamics at the core of the quantum dot to account for the nonlinear effects and lattice statics Green's function for the host lattice. The lattice statics Green's function reduces asymptotically to the continuum Green's function which we use to model the free surface. The model is applied to Ge quantum dots of realistic sizes up to 6.5 nm buried in Si containing a free surface. The topography of the free surface and the strain field are calculated which can be measured and used to characterize the QD. We have also calculated the strain energy of a quantum dot which is useful for predicting the formation of arrays of quantum dots and for strain engineering of quantum dots.

1. INTRODUCTION

Currently there is a strong interest in modeling the mechanical characteristics of quantum dots (QDs) in semiconductors because of their potential application in powerful new devices like huge memory systems, ultra low threshold lasers, and quantum computers. A QD causes lattice distortion in the host solid which manifests as strain and displacement field throughout the solid.

Strains and displacement field at a free surface in the solid can be measured and used to characterize the QD. Strain field determines the elastic energy of the system and is mainly responsible for the formation of arrays of QDs. The strain energies provide an indication of which positions may be favorable for formation of neighboring dots in self-assembled arrays. Also, the surface distortions are useful for relating scanned-probe microscopy observations to dot size and position. The strain and displacement field are essentially continuum-model parameter whereas the lattice distortions are discrete variables that must be calculated by using a discrete lattice theory. Hence one needs a

multiscale model that relates the discrete lattice distortions at the microscopic scale to a macroscopic parameter such as strain.

A QD has to be modeled at the following scales: (i) the core region (sub-nanometer) inside the QD where the nonlinear effects may be significant, (ii) the region of the host solid around the QD (nanometer), and (iii) free surfaces and interfaces in the host solid (macro scale).

A mathematical model for a nanostructure should account for at least one free surface in the solid since the measurements are usually made at or near a free surface. The model should satisfy the following criteria: (i) it must account for the discrete structure of the lattice in and around the nanostructure and, therefore, the crystallite must be sufficiently larger than the nanostructure, (ii) the crystallite must be large enough to include a free surface and for the lattice distortions to smear out into a continuum, so that the continuum parameters like the strain and the displacement fields can be defined, (iii) the continuum parameters have to account for the elastic anisotropy since most materials of practical interest are anisotropic, (iii) the model must include nonlinear interactions between atoms inside and close to the nanostructure even if the host lattice is harmonic, and, finally, (iv) the model should be computationally efficient.

A pure continuum model of a QD yields useful results in the far field but is not valid close to the QD. An excellent review of the continuum model calculations for QDs is given by Jain et. al. [1] and of multiscale models by Ortig and Phillips [2]. The lattice statics Green's function (LSGF) method [3] is computationally efficient and can model large crystallites but does not account for the nonlinear interactions. Molecular dynamics (MD) accounts for nonlinear forces but is usually limited to crystallites of only a few hundred atoms. For a review of modeling at different scales and other references, see [2].

We have developed a method which integrates the MD, LSGF, and anisotropic continuum Green's function (CGF) for modeling QDs. In our method the core of the defect or the nanostructure, where the nonlinear effects are significant, is modeled by using MD. This is the sub-nanometer scale region including a few hundred to a few thousand atoms which can be easily handled by MD. The core is surrounded by a shell to which the core atoms are pegged in the MD calculations. The lattice beyond the core is modeled by using the LSGF method. This integrated method has the advantages of both the techniques. It models a large crystallite and includes nonlinear effects in the core without excessive computational requirements. The LSGF reduces to the CGF at large distances from the core. The CGF is then used to model a free surface as in the Mindlin problem [4,5]. Thus our model integrates MD, LSGF, and CGF and bridges the length scales from nano to macro.

Our method which we call the MDGF method, is computationally efficient since powerful techniques for calculating LSGF and CGF are available in the literature [2]. This method enables us to model a large realistic size Ge QD (6.5 nm) in a host containing two million atoms. We have applied the MDGF method to model a 6.5 nm Ge QD in a semi-infinite Si containing 2 million atoms. Here we report our results on the strain field at the free surface of the host. Detailed results will be published elsewhere.

2. MULTISCALE MODEL OF A QD

The basic formulation of the multiscale Green's function method has been described in [4,5]. Here we only give the results. The atomic displacements **u** in a solid containing defects are given by [3] the matrix equation

$$\mathbf{u} = \mathbf{G^*F} = \mathbf{GF^*(u)}, \qquad (1)$$

where **G*** is the defect Green's function of the solid containing a QD; **G** is the perfect lattice Green's function; **F** is the force at the initial atomic positions; and **F*(u)** is the Kanzaki force which is a function of **u** and the interatomic potential. The matrices **u**, **F**, and **F*** are column matrices and **G** and **G*** are square matrices in the vector space of lattice sites.

In order to solve Eq. (1), we divide our model crystallite in 3 regions: core, shell, and host. The core region itself consists of an inner core consists of the foreign atoms constituting the QD and an outer core consisting of host atoms. The shell and the host regions consist of only the host atoms. Thus we can treat the core region as a defect in the host solid. The thickness of the outer core is taken to be more than the range of the interatomic potential between the QD atoms and the host atoms so that the QD atoms do not directly interact with the shell atoms.

The core regions are modeled by using MD with the shell region treated as fixed which provide the necessary boundary conditions for MD calculation. The core displacements calculated by MD, exert a force on the shell atoms which are not moved by MD. Using these forces, the displacements in the shell and the host regions are calculated by using the LSGF. The MD calculations are then repeated corresponding to the new positions of the shell atoms. Equation (1) is thus solved by iteration until the net force on the shell atoms is zero.

We consider a semi-infinite solid and introduce a surface in the host region using the technique described previously [5] which depends upon the use of Kanzaki forces in the Mindlin problem. We have not accounted for the effect of the surface on the Kanzaki forces. This introduces a small error into our results for surface strains and displacements, which is not expected to affect our general conclusions.

We have applied our formulation to model a Ge QD in Si. For the interatomic potential, we have chosen the modified embedded atom model (MEAM) [6] with modified parameters. The LSGF is calculated using the Fourier transform technique [3] in a Born von Karman supercell containing 10^6 unit cells or 2×10^6 atoms. The MD calculations used the XMD computer program, described by Rifkin [7], significantly modified by the addition of the MEAM potential. The QD is contained within a supercell with full Wigner-Seitz face-centered-cubic symmetry. The supercell boundaries remain fixed throughout the solution procedure. The supercell diameter is 34.2 nm. Therefore we expect to obtain good accuracy for atomic displacements and derived quantities up to a distance of about 17 nm from the center of our QD. By this distance, the displacements

and strains are very small. The Kanzaki forces, which occur near the center of the supercell and therefore are considered to be unaffected by the cell boundary, are used to evaluate displacements and strains at much larger distances. Our Ge QD is built up by including atoms out to spherical cutoffs, but subject to the symmetry of the lattice.

In the present calculations the QD is assumed to have the full cubic symmetry, but this is not a constraint on the method. The QD contains 7193 Ge atoms which constitute the inner core, for a QD diameter of about 6.5 nm. The outer core contains 26340 atoms. The shell consists of 7796 Si atoms. This size was chosen because it is large enough to be physically realistic but still small enough to be modeled with tractable calculation times.

3. RESULTS

We have calculated surface displacements and strains due to QDs of different sizes. Each QD has the shape of the Wigner Seitz cell of the host lattice which is nearly spherical for large QDs. The approximate radii of the QDs ranged from 4 to 24 in units of a/4 where a = 0.5432 nm is the lattice constant of the Si lattice. The largest size of radius 24 is labeled as size F. We find that the surface displacements of size F are of a magnitude sufficient to be observed by advanced scanned probe microscopy. The smallest QD nearest the surface produce a characteristic pattern of out-of-plane surface displacement, namely, a depression or indent at the center of the peak. This feature gradually decreases in magnitude as the dot size increases, and is absent in the largest dot.

Due to limitations of space, we give here in Fig. 1 only the results for strain energy and hydrostatic strain due to a QD of size F. Both the strain energy at the surface and the hydrostatic strain, given as the trace of the strain tensor, reveal patterns of spatial dependence similar to surface displacements discussed in the preceding paragraph. A key point is that the hydrostatic strain at the surface is tensile, in contrast to the strain in the infinite solid near the QD. The hydrostatic strain becomes negative in the far-field. The negative hydrostatic strains occur where the compressive radial (from the QD center) strain becomes larger than the tensile tangential (relative to the QD center) strain. This is a far-field effect.

Figure 1 shows that the maximum of the two curves occurs directly above the QD. According to the simple model given by Tersoff et al. [8], the surface strains can be used to estimate the tendency for self-alignment of an added layer of QD on top of an existing layer. In this simple model, the favored growth should “reduce the mismatch” but accurate predictions of QD array formation would require calculations of the elastic interaction energy between dots or of the elastic energy release rate [9], which are beyond the scope of the present paper. Our results on surface strains and strain energy densities, as given in Fig. 1, show that the strains at the surface are all tensile. The Ge atom is larger than the Si atom, so a Ge atom incorporated into a tensile strain field should reduce the mismatch. We see that the maximum of tensile strain is directly above the QD. Hence we would expect the next QD to form in the vertical position, directly above the existing QD. However, the situation is different for the small QD. In this situation, the maximum strain is not directly above the existing QD, but is offset. So, based on the model of [8],

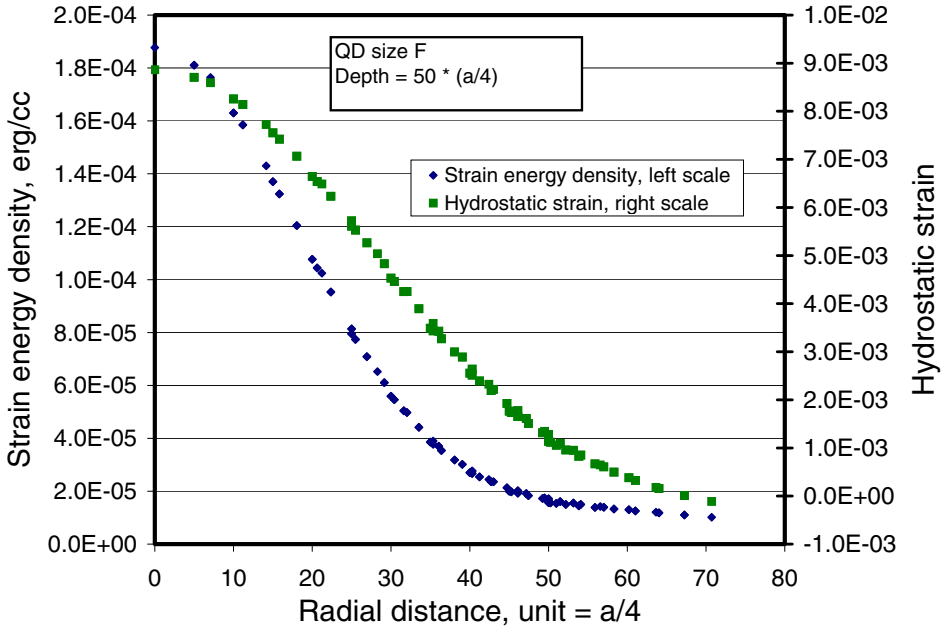

Figure 1. Strain energy density and hydrostatic strain on the surface above QD size F, depth 50 (a/4).

one would suspect that growth of vertical arrays should break down, or be less favored, for very small QD close to the surface.

Calculations of the displacements around Ge-Si QD of various types have been reported by Makeev and Madhukar [10]. Their fully atomistic calculation used a different interatomic potential, and they reported results in terms of stresses and strains. Their MD calculation included a free surface, but without modifying the potential at the surface, and without allowing the surface to reconstruct. Their extraction of stress and strain values from atomic displacements required a choice of definitions for taking the continuum limit of functions of discrete variables. Here we treat the surface in the continuum approximation, using the continuum GF as the asymptotic limit of the LSGF. One advantage of this method is that the limit is unique [4] and not subject to arbitrariness introduced by different choices of taking the limit. Our atomistic treatment extends much further into the substrate. The present results, like those of [10], reproduce the general scaling of the elasticity solutions and show that the free surface above a Ge QD in Si is displaced out of plane, in a direction away from the QD, meaning that the QD produces a broad peak on the surface.

4. CONCLUSIONS

We have developed a computationally efficient multiscale model for QDs in semiconductors and applied it to calculate the displacement field, strains, and strain energy of a 6.5 nm Ge QD in semi-infinite Si containing 2 million atoms. The model seamlessly bridges the length scales from nano to macro by combining MD, LSGF, and anisotropic CGF.

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