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Atomistic Computation of Local Stress and Strain Distribution around an InAs Quantum Dot between a GaAs Capping Layer and a Substrate

Eun Cheol Do and Byeong-Joo Lee*

Department of Materials Science and Engineering,
Pohang University of Science and Technology, Pohang 790-784, Korea

The utilization of self-assembling phenomena is important in nano material processes. For the fabrication of well-aligned multilayered nanodots or nanowires, it is necessary to know the atomistic strain/stress distribution in the capping layer. In the present study, an atomistic computational approach based on an modified embedded-atom method (MEAM) interatomic potential is used to investigate the atomistic strain/stress distribution in a GaAs capping layer over an InAs quantum dot (QD) on a GaAs substrate. The atomic scale local strain/stress around the QD can be well predicted by atomistic simulation and the approach can be used to determine the optimum interlayer distances for well-aligned multilayered QDs.

Keywords: InAs/GaAs quantum dots, strain/stress distribution, MEAM, atomistic simulation

1. INTRODUCTION

A great amount of research effort is being made on infrared photo detectors, light-emitting diodes, laser diodes and memory devices based on self-organized quantum dots (QDs).[1-3] The misfit stress around a QD plays a decisive role in the evolution of the shape and vertical alignment of QDs[4] and also has a great effect on the energy bandgap structure of QD[5,6] during and after their formation. Analysis of the local stress distribution around a QD is therefore essential for successful fabrication of QD structures.

Experimental techniques such as TEM and XRD have been used for the stress analysis around QDs.[7-9] However, accurate analysis of the stress distribution around a nano-sized QD embedded in a substrate and capping layer is not easy. A finite-element-method based on continuum mechanics and atomistic approaches such as molecular dynamics have been be used as computational techniques.[5,10,11] The approach based on continuum mechanics has limited applicability because the behavior of individual atoms is thought to be decisive in the structural evolution of nano-sized materials. In atomistic approaches, the decisive factor is the reliability of the interatomic potential.

The first-principles calculations provide the most reliable interatomic potentials for atomistic simulations. However, due to the limitation of size (or the number of atoms), it is often not possible to investigate the material behaviors solely by using the first-principles calculations. Note here that the number of atoms in a 10 nm to 20 nm QD can reach several hundred thousands. Another approach is to use (semi-) empirical interatomic potentials that can deal with more than a million atoms.

An interatomic potential that can reproduce various physical properties of relevant elements correctly should be used to obtain physically meaningful results from atomistic simulations based on (semi) empirical interatomic potentials. Moreover, a common potential formalism should be used to describe individual elements as a way of dealing with multicomponent systems composed of elements with different equilibrium structures. Unfortunately, however, most of the presently available many-body interatomic potential formalisms are mainly for a limited range of elements.

Because of the difficulty in developing interatomic potentials, atomistic simulations have been carried out mainly for simple systems such as the Ge/Si QD; they have rarely been used for multicomponent compound semiconductor systems, such as InAs/GaAs or InN/GaN QDs. As an interatomic potential formalism for atomistic simulations on multicomponent systems, the modified embedded-atom method[12] (MEAM) potential is highly recommended because it can cover a wide range of elements (fcc, bcc, hcp, diamond and even gaseous elements) with a common formalism and functional form. The MEAM was created by Baskes,[12] by modifying the EAM,[13,14] to include the directionality of bonding. In the original MEAM,[12] only interactions among the first nearest-neighbor atoms were considered. Recently, the MEAM was modified once again by Lee and Baskes[15,16] to consider partially the second nearest-neighbor atom interac-

*Corresponding author: calphad@postech.ac.kr

tions and to remove some critical shortcomings in the original MEAM. The generalized MEAM (the second nearest-neighbor or 2NN MEAM) has been applied to a wide range of elements including bcc,[16] fcc[17] and hcp[18] metals, carbon,[19] silicon,[20] germanium,[21] indium[22] and higher order systems between different types of elements, such as Fe-C,[23] Fe-N,[24] Fe-H,[25] Ga-In-As[26] and Ga-In-N[27] systems.

With the developed MEAM interatomic potential,[26] atomistic computations on the Ga-In-As system is now feasible. The purpose of the present study is to analyze the local stress and strain distribution around an InAs QD embedded between a GaAs substrate and a capping layer. The agreement between the calculated and experimentally measured local strain distribution around a QD demonstrates the applicability of the atomistic computational approaches for determining the optimum interlayer distances in the fabrication of well-aligned multilayer QDs in $Ga_{1-x}In_xAs$/GaAs QD systems.

2. SIMULATION METHOD

2.1. Interatomic Potential

In MEAM, the total energy of a system is approximated as,

$$E = \sum_i \left[F_i(\bar{\rho}_i) + \frac{1}{2} \sum_{j(\neq i)} \phi_{ij}(R_{ij}) \right] \quad (1)$$

where F_i is the embedding function for an atom i embedded in a background electron density $\bar{\rho}_i$, and $\phi_{ij}(R_{ij})$ is the pair interaction between atoms i and j separated by a distance R_{ij}. For the energy calculations, the functional forms for F_i and ϕ_{ij} should be given. The background electron density at each atomic site is computed by combining several partial electron density terms for different angular contributions. A specific form is given to the embedding function F_i, but not to the pair interaction ϕ_{ij}. Instead, a reference structure where individual atoms are on the exact lattice points is defined and the total energy per atom of the reference structure is estimated from the zero-temperature universal equation of state given by Rose *et al.*[28] The value of the pair interaction is then evaluated from the known values of the total energy per atom and the embedding energy, as a function of the nearest-neighbor distance.

Before an alloy system can be described, the pair interaction between different elements should be determined. For this, a technique similar to that used to determine the pair interaction for pure elements is applied to binary alloy systems.[12] That is, a binary reference structure is chosen. The total energy per atom of the reference structure is computed by using once again the universal equation of state. The pair interaction between different elements is then obtained from the known values of the total energy per atom and the embedding energy of the reference structure. The MEAM formalism for pure elements and binary systems is fully documented in the literature[12,15-27] and is not be repeated here.

Table 1. Physical properties of the Zincblende-type InAs and GaAs calculated using the MEAM interatomic potential: cohesive energy, E_c (eV), lattice parameter, a (Å), elastic constants, C_{11}, C_{12} and C_{44} (10^{12} dyne/cm^2), and bulk modulus, B (10^{12} dyne/cm^2)

	InAs		GaAs	
	Exp.	MEAM	Exp.	MEAM
E_c	2.986	2.986	3.165	3.165
a	6.058	6.036	5.653	5.653
C_{11}	0.833	0.835	1.189	1.182
C_{12}	0.453	0.451	0.502	0.53
C_{44}	0.396	0.392	0.614	0.598
B	0.580	0.580	0.748	0.748

By way of example, Table 1 compares the calculated physical properties of GaAs and InAs with experimental data.

2.2. Sample Preparation

A sample with an embedded InAs QD between the GaAs substrate and the capping layer was prepared for the computation of stress and strain distribution around a QD. Figure 1 shows the size, structure and crystallographic orientation of the InAs QD on the GaAs substrate. The QD has a dome shape and its size is close to the typical size of QDs.[9] Even though a periodic boundary condition was applied into the planar directions (x and y directions in Fig. 1) of the substrate, the sample size in those directions was kept the same as that of a pure substrate material. After the QD was set on the substrate, the sample was covered with a capping layer made of the same material as the substrate. The sample was then fully relaxed at 0 K. When the relaxation was finished, the local strain and stress of individual atoms were calculated.

2.3. Calculation of the Local Stress and Strain

The atomistic simulation provides information on the location and stress tensor of individual atoms. The strain of individual atoms is calculated by comparing the nearest-neighbor bonding distance of each atom with that of perfect crystal. The hydrostatic strain is calculated by summing all three dimensional components of the strain between one atom and neighboring atoms. The planar or vertical strain can also be calculated by selecting the components. The same calculation (namely the calculation of hydrostatic, planar and vertical stress) can also be made for the local stress.

3. RESULTS AND DISCUSSION

A recent TEM study[9] on the InAs/GaAs QD system reported that vertically well-aligned multilayered QDs can be fabricated with an interlayer distance of 9 nm whereas the

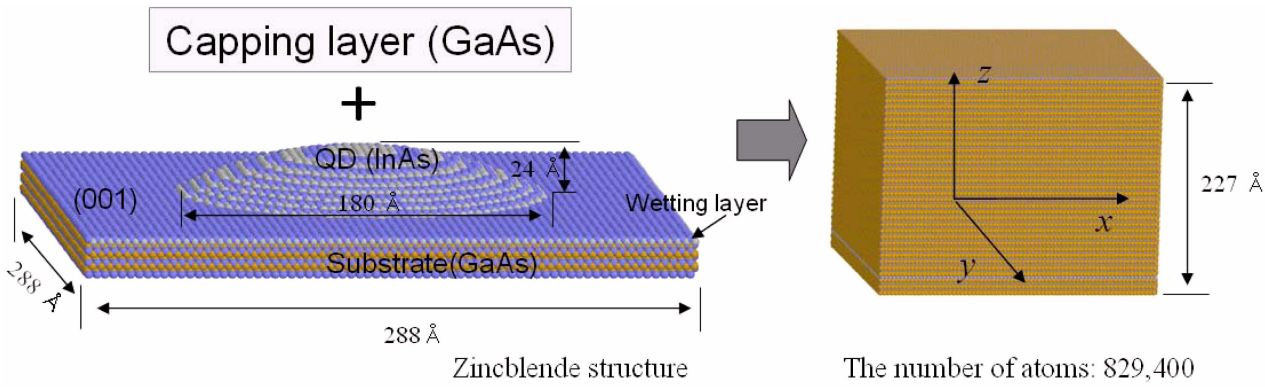

Fig. 1. Schematic drawing of a QD and the capping layer for simulation.

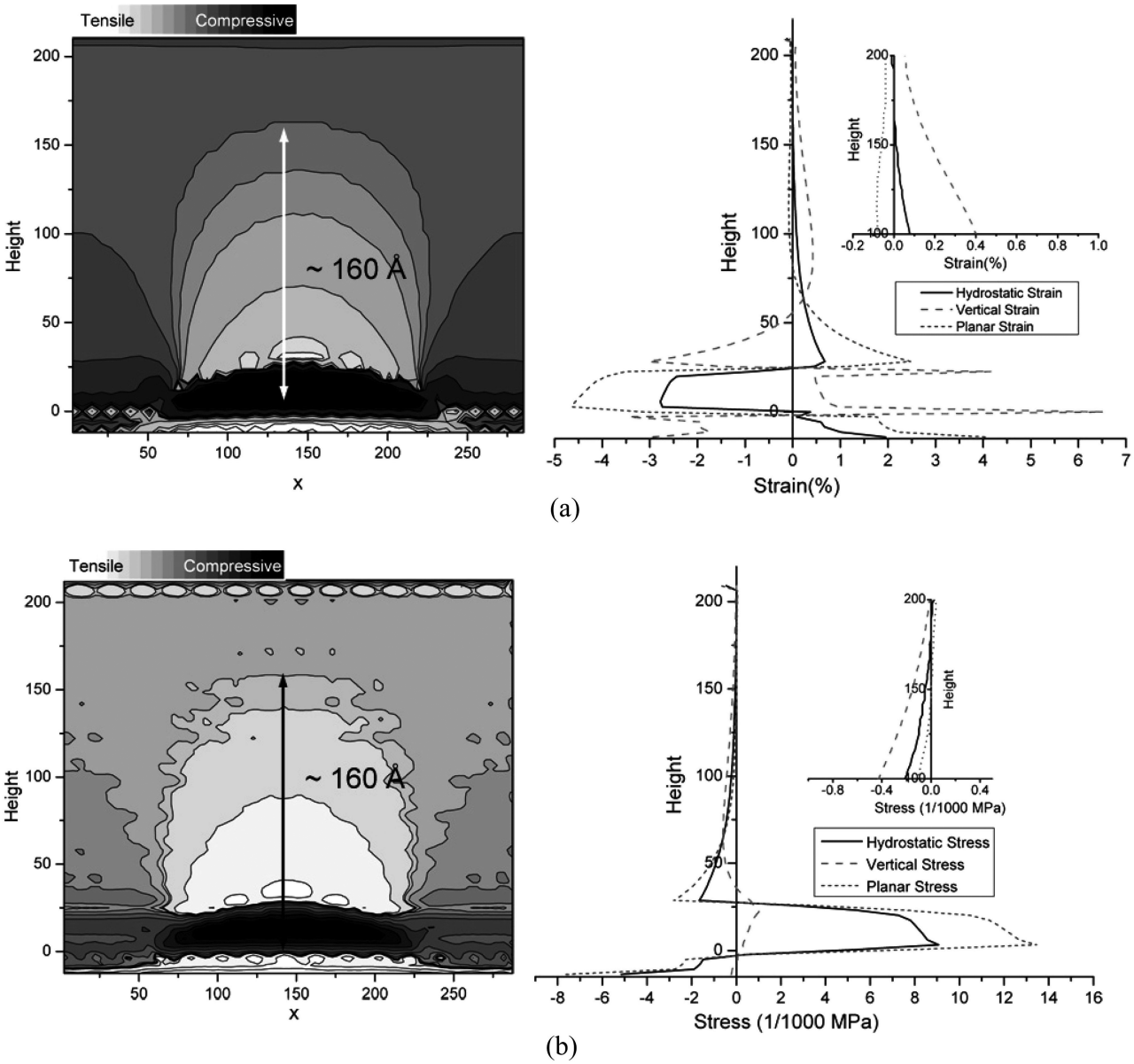

Fig. 2. Hydrostatic (a) strain and (b) stress distribution around an InAs QD embedded between a GaAs substrate and a capping layer. The vertical and planar components of the strain/stress are plotted on the right.

well-alignment is not obtained when the distance is 15 nm. Furthermore, the local strain around an InAs QD with a diameter of about 20 nm between the GaAs capping and substrate layers was found to remain up to about 15 nm from the substrate. Given that the misfit strain or stress around a QD plays a decisive role in the evolution of the shape and vertical alignment of QDs, attention was focused on how well the atomistic computation can predict the local strain/stress distribution around a QD and can describe the way in which the alignment of the QDs depends on the interlayer distance.

Figure 2 shows the calculated local strain and stress distribution on the vertical section at the center of the InAs/GaAs QD system. On the left is the distribution of the hydrostatic component. The color (white or black) represents the state of the strain or stress (tensile or compressive). On the right, the planar and vertical components, as well as the hydrostatic component along the vertical line at the center of the QD, are plotted as a function of distance from the substrate. Both the hydrostatic strain and stress are shown to propagate up to about 160 Å from the substrate. The corresponding experimental value[9] was about 150 Å. The close agreement in the range of the local strain between the experiment and calculation indicates the reliability of the MEAM interatomic potential and the applicability of the atomistic calculation approach.

The residual strain/stress (especially the planar component) on the surface of the capping layer is believed to have a critical effect on the nucleation of QDs on the next layer. For a good vertical alignment of multilayered QDs, some residual strain or stress is thought to be needed on the surface of the capping layer. The right-hand side of Fig. 2 shows that the planar component of the residual strain/stress disappears at a range of 8 nm to 13 nm from the substrate along the center of the alignment. On the basis of this result, the formation and failure of the vertically well-aligned multilayered QDs with an interlayer distance of 9 nm and 15 nm, respectively, can be rationalized.

This study confirms that the atomic-scale local strain/stress around a QD can be well predicted by atomistic simulations and can be used to determine the optimum size of the interlayer distance for a well-aligned multilayered QD system. Similar calculations can also be performed for InN/GaN or Ge/Si QDs with the aid of readily developed MEAM potentials.[20,21,27] The variance in bonding distances or lattice parameters with the composition of the $Ga_{1-x}In_xN$/GaN or $Ge_{1-x}Si_x$/Si QD system is correctly reproduced by the atomistic calculation. Thus, the atomistic approach can also be applied to multicomponent QD systems with various dot compositions.

4. CONCLUSIONS

The atomic-scale local strain/stress around an InAs QD embedded between a GaAs substrate and a capping layer can be well predicted by an atomistic simulation based on the MEAM interatomic potential. The atomistic approach can be used to determine the optimum interlayer distances for well-aligned multilayered QD systems. The MEAM atomistic approach is also applicable to $Ga_{1-x}In_xN$/GaN and $Ge_{1-x}Si_x$/Si QD systems.

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