Stress distribution, strains and energetics of Si-capped Ge quantum dots: An atomistic simulation study

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Abstract. We study Si-capped Ge quantum dots which are very interesting as these nanostructures emit/absorb light in the near infrared and visible. Their preparation proceeds by the deposition of Ge on Si, which forms small islands. By successive deposition of Si and Ge, a periodic structure is formed in three dimensions, of Si-capped Ge (QD’s). Experimentally it has been found that these QDs have different shapes and sizes, which are strongly dependent on their preparation conditions and method. For our study we created atomistic models representing nanostructures consisting from a few hundreds to tens of thousands atoms of Si where a portion of them replaced with Ge atoms. The replaced atoms were selected in order the Ge atoms to form small islands shaped in pyramids or domes and with different sizes. This nanostructure was repeated periodically in three dimensions, forming finally a periodic QD structure. For these structures we used the Stillinger-Weber interatomic potential models to relax them to the minimum total energy. Then we studied the strains distribution and energetics and their dependence on the substrate composition and the alignment of the QD along the growth direction. It is found that the distribution of the strains differ compared to an equivalent alloy, with the Ge atoms having a broader one, there is a buffer layer composition for which that nanostructure has the lowest energy and the distribution of strains are proportionally divided in the Ge and Si atoms, and that the alignment along the growth axis with the lowest energy corresponds to each QD on top of the next one.

1. Introduction
Over the last years nanostructures have gained a high interest both scientifically and for technology. The special properties of these structures have propelled the research and development. A lot of such structures have been produced and studied, although a huge variety of possible structures remains to be studied. An important point about nanostructures is the uniqueness of each structure and the strong dependence between geometry, structure and properties. A class of very interesting nanostructures is that of quantum dots (QD) of semiconductor materials. One way to form QDs is to exploit the lattice mismatch of the different materials [1], which are used in growing compounds with alternate deposition on a substrate. These nanostructures have shown special optical and electronic properties [2, 3] and have already found applications in optoelectronics. A lot of different materials and processes are used in the production of QDs, and these determine their shape and properties. A special case of QDs is that of Si-capped Ge QDs. These structures are developed with the periodic deposition of a few monolayers of Ge, and their capping with a thicker layer of Si. In this way the Ge atoms form small islands because of the lattice mismatch. The shape of QDs can be pyramid-like or dome-like, and it depends mainly on the thickness of the capping Si layer [1, 4] and the annealing process, while their size varies from a few nm (ultra small) to hundreds of nm. Many nanostructures are grown on
substrates, where first a buffer layer is deposited, usually an alloy. For the case of Ge QDs this buffer layer is a Si$_{1-X}$Ge$_X$ alloy. The composition of the buffer influences the strains and therefore the final properties of the QDs [5]. The purpose of the present work is to study theoretically the energetics and the strains induced inside QD structures and in relation to the buffer layer composition and to the relative alignment of QDs.

2. Method

The general idea is to create an atomistic model structure simulating a real QD, with the desirable size and shape and to relax this structure to the minimum energy. For this purpose someone can use an appropriate empirical Interatomic Potential Model (IPM). For the case of materials we study, there are numerous of available empirical IPM. One of the most widely used is the Stillinger-Weber (SW) [6]. Another model also widely used is the Keating model [7] which is accurate only for small distortions. Both models consist of two- and three- body terms and have the general form of equation 1.

$$E(\{\hat{R}_i\}) = \sum_{\{i,j\}} u_2(\hat{R}_i, \hat{R}_j) + \sum_{\{i,j,k\}} u_3(\hat{R}_i, \hat{R}_j, \hat{R}_k),$$  

(1)

Where $u_2(\hat{R}_i, \hat{R}_j)$ is the two-body term between atoms $i$ and $j$ and $u_3(\hat{R}_i, \hat{R}_j, \hat{R}_k)$ is the three-body term of atoms $i$, $j$ and $k$. Here we used the SW model that penalizes any deviation from the ideal diamond structure bond angle in the three-body term and it is effective for moderate distortions. The SW model uses a set of empirically fitted parameters [6]. We have utilized STREL windows application which we developed and it is a versatile computing environment for the creation of atomistic model structures, the relaxation of these structures under different controlled conditions, the visualization of the interested stress and energetic parameters and finally the calculation of electronic structure and the optical properties. For this work we assume that the structures are relaxed if the maximum force is less than $10^{-5}$ eV/Å.

In figures 1 and 2 a visualization of two of the structures we used in this work is presented, where the Ge atoms are emphasized by representing them by much bigger spheres than Si atoms. In the figure 1 the formed QD is a small pyramid with 343 atoms of Ge and 31657 Si atoms to a total of 32000 atoms. In the figure 2 the formed QD is a dome with 447 atoms of Ge and 15553 Si atoms to a total of 16000 atoms. The periodic repetition of these structures produced a 3D array of Si-capped Ge QDs.

3. Results

Here we studied the distribution of strain in QDs and energetics in relation to buffer layer composition
and to alignment of QDs along the growth direction (stacking). In all cases the structures were relaxed
to their minimum total energy. Also in the studies of strain distribution and buffer layer energy
dependence, the dots are considered to be perfectly aligned one on top of the other. The interdiffusion
at the Si/Ge interface has not been taken into account. This interdiffusion is expected to affect the
strains of certain atoms, as preliminary results show and it will be the subject of a later work.

3.1. Strain distribution
In figure 3 there is a histogram of strains of the structure in figure 2 relaxed on Si buffer. In this
histogram we can distinguish several groups of atoms with similar strains. First, the majority of Si
atoms (about 80%) have been compressed or expanded by less than 0.1%. Next a 2.5% of Si atoms
have been expanded by more than 0.4% and this is the group of Si that interfaces to QD. Another 5%
of Si atoms have been expanded by less than 0.5% and these atoms are vertically positioned over and
under the QD but leaving about 4 monolayers (ML) of Si atoms compressed by 0.1% to 0.4%. In the
same category belong the remaining 10% of Si atoms that occupies the corners of the structure just
below and over the QD. For the Ge atoms, all are compressed compared to their optimum tetrahedron
volume and form 2 main groups. That belonging to the interface with Si atoms and having been
compressed by more than 4.5% which are a portion of 35% and the rest 65% belonging to the core of
the QD that have been compressed by 2.5% to 4.5%. By comparison with an alloy of the same
composition Ge atoms are less strained by a factor of two.

Figure 3. Strain
distribution of the dome
in figure 2 as exported
by the STREL
environment. The upper
part shows the strains
of Ge while the lower
the strains of Si atoms.

Figure 4. Energy per
atom versus buffer
composition for a dome
with 3553 Si atoms and
447 Ge atoms.
3.2. Buffer layer
In the case of Si-capped Ge QDs as a buffer layer is used an alloy of the form Si$_{1-X}$Ge$_X$. In Figure 4 we plot the energy per atom of a structure similar to that of figure 2, but with 4000 atoms in total, in relation to the buffer layer composition. The inset is a magnification of the leftmost part of the main graph, where we observe that for some stoichiometry the energy per atom has a minimum. As the strain distribution depends on the buffer composition it is interesting to note that the minimum energy corresponds to the strain symmetrized case.

3.3. Stacking
Another studied parameter here is the alignment of the QDs along the growth direction. To study this we calculated the total energy or the energy per atom of relaxed structures when the dots do not aligned vertically but show a shift along the X or Y axis. The results are shown in figure 5. We observe that the structure has the lowest energy when the dots are aligned one on top of the other along the growth axis.

![Figure 5. Energy per atom versus vertical misalignment of QDs.](image)

4. Conclusions
We have produced atomistic models of 3D periodic arrays of Si-capped Ge QDs and studied the strains, strains distribution and their dependence on the buffer layer composition and QD alignment along the growth direction. We find that the distribution of the strains differ compared to an equivalent alloy, with the Ge atoms having a broader one, there is a buffer layer composition for which that nanostructure has the lowest energy and the distribution of strains are proportionally divided in the Ge and Si atoms, and that the alignment along the growth axis with the lowest energy corresponds to each QD on top of the next one.

5. References
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