Bandstructure calculations of strained nanostructures via atomistic pseudopotential methods

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INTRODUCTION

Electronic and transport properties of confined nanostructures as quantum wells, nanowires and nanodots fabricated in heterostructures as Si/Ge or III-V compounds are strongly dependent on quantum confinement and strained configurations. Here, we present a rigorous approach to compute electronic properties of strained nanostructures based on an atomistic empirical pseudopotential method (AEPM).

METHODS AND RESULTS

This method extends the use of EPM [1] to atomistic supercells of confined structures, allowing a natural comparison with other atomistic models. With respect to other empirical methods as the tight-binding (TB) model, the AEPM depends on a very small number of parameters, the Fourier coefficients of the ionic potential $V_{\mathbf{G}} = S_{\mathbf{G}} \sum_{\alpha} v_{\alpha}(\mathbf{G})$, where $S_{\mathbf{G}}$ is the form factor and $v_{\alpha}(\mathbf{G})$ is the potential of the ion α and $\mathbf{G}$ is the reciprocal wave vector.

Fig. 1 shows the bandstructure of bulg Ge as calculated by TB model and atomistic EPM model. In Fig. 2 we show the supercell considered as a first application of the method. It consists in a Si/sGe/Si epitaxial heterostructure, which forms a [001]-oriented quantum well. In our approach the strain induced by the lattice mismatch between the two materials is naturally included by computing the form factors of atoms properly relaxed. To this purpose, the atomic displacement due to the surface relaxation was calculated by means of an empirical valence force field model. The corresponding stress level along the confinement direction is plotted in Fig. 3. Fig. 4 illustrates the ability of the AEPM in describing at the atomic scale the total wave function of the system.

By solving the Schrödinger problem for the Hamiltonian obtained from the AEPM, we extracted the bandstructure of the Si/sGe/Si compund and compared it with the results given by a $sp^3d^5s^*$ TB model [2][3][4]. Author would like to point out that both models are calibrated on the same *ab initio* material and lead to consistent results in terms of effective mass and bandgap. In Fig. 5 we reported a relatively good matching between the two models. Fig. 6 shows the bandstructures computed by our AEPM for Ge layers of different thickness. As expected, we found a reduction of the energy gap as far as the quantum confinement is reduced.

CONCLUSION AND PERSPECTIVES

Accurate bandstructure calculations of a Si/sGe/Si heterostructure have been performed by means of atomistic pseudopotential methods. Further applications will concern different types of 2-D and 1-D systems as fully-depleted MOS and nanowire transistors.

ACKNOWLEDGMENT

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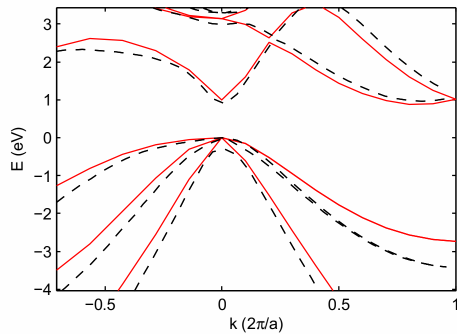

Fig. 1. Band structure of bulk Ge. Black dashed lines are the result of TB simulations. Red lines are the result of atomistic EPM simulations.

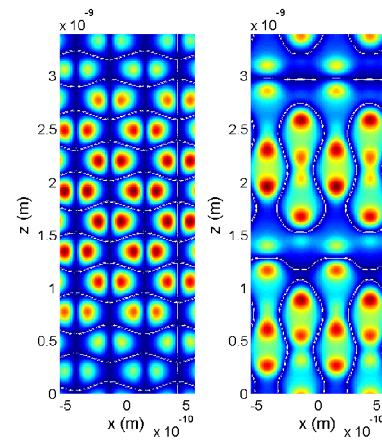

Fig. 4. Gradient plot of the wave-function of the lowest conduction (right) and of the highest valence (left) subbands.

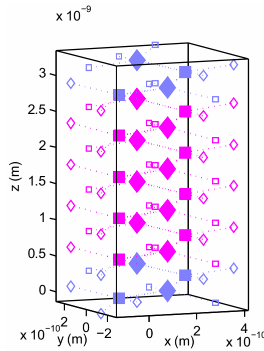

Fig. 2. Supercell structure of a Si/sGe/si heterostructure with a channel thickness $T_{\mathrm{Ge}} \approx 2$ nm. Ge atoms are red and Si atoms are blue.

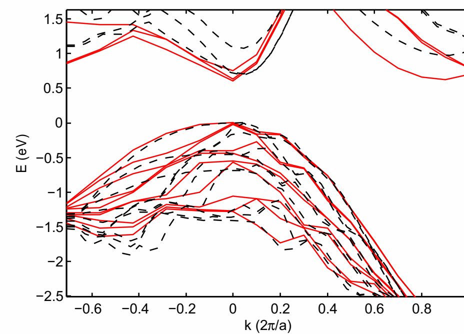

Fig. 5. Band structure of the Si/sGe/Si heterostructure of Fig. 2. Black dashed lines are the result of TB simulations. Red lines are the result of atomistic EPM simulations.

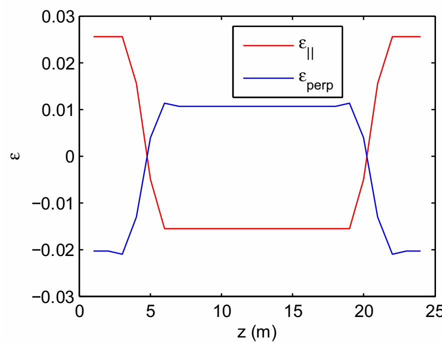

Fig. 3. Spatial profile of stress level for the supercell of Fig. 2, calculated by a valance field force Keating model.

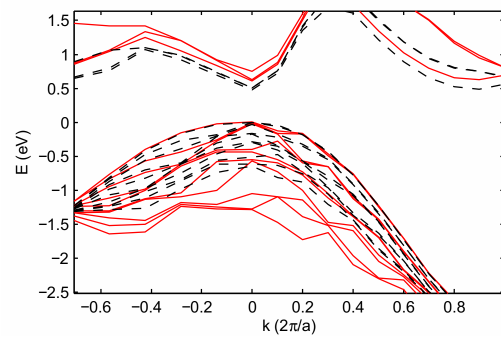

Fig. 6. Band structure of the Si/sGe/Si heterostructure with AEPM for different Ge layer thickness (red lines for T_{Ge}= 2 nm and dashed black line for T_{Ge}= 4 nm).