Thermal transport across strain relaxed Si/Ge interfaces

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INTRODUCTION

Semiconductor superlattices are widely used and studied in thermoelectric and optoelectronic devices. The thermoelectric figure of merit depends on both electrons and phonons. Control of electron and phonon transport across the interface is important because it influences device thermal performance. *Ab initio* methods are often adopted in the study of nano-structures, but they tend to be computationally intensive and are appropriate only for small systems.

In this paper, new atomistic models are established for the requirement of realistic nano device modeling. To be specific, Empirical Tight-Binding (ETB) method is adopted in the electron band structure calculation. Valence Force Field (VFF) Keating model is used to produce the phonon dispersion relation. These two methods are capable to simulate the real size device. The strain relaxation which is important for heterostructures is typically ignored in literature. In this paper, Keating strain model is used to relax the SiGe interface to make sure that the structure is stable. Nonequilibrium Green's Function method (NEGF) in atomistic representations are applied to calculate the transport in both electron and phonon case [1].

MODEL

Electrons are atomically represented in a 20 band ETB model [2], while the atomic VFF Keating model is used to represent the phonons [3]. In the case of Si/Ge interfaces, all atom positions are relaxed to minimize the total elastic strain energy of the lattice [4]. These atom positions influence the phonon dispersion via the dynamical matrix resulting from the device strain relaxation as well as the electronic Hamiltonian via the strain model of Boykin et al. [2]. The nonequilibrium Green's functions for the electrons and phonons in the relaxed device structure are solved with NEMO5 to predict the ballistic electron and phonon heat transport properties [5].

RESULTS AND DISCUSSION

To illustrate the relaxation of the atoms, Fig.1 shows the strain component ε_xx of a 1.08nm thick Ge quantum well embedded in homogeneous Si after the strain relaxation calculation. Since the Ge well in this example is very thin, the Ge well is strained to adapt to the Si lattice. Figure 2 compares the phonon transmission of the relaxed Ge quantum well with the unrelaxed structure and the pure Si and Ge transmissions, respectively. It is obvious that the well transmission cannot be derived from results of the homogeneous material. The relaxation of the interface creates an effective reflecting potential which reduces the transmission. This reduction is a function of energy and cannot be predicted without explicit numerical calculation.

Figure 3 shows the thermal conductance in both electron and phonon case. The interface relaxation of the heterostructure reduces the thermal conductance of both electrons and phonons. Depending on the temperature, on the material and on the device geometry, the impact of the interface relaxation on electron and phonon transmission varies.

Similarly, the phonon transmission is reduced by the interface relaxation in the case of Si/Ge/Si nanowires: Figure 4 illustrates the strain component ε_xx for a squared Si nanowire of thickness 6 nm with a 1.2 nm thick Ge layer. Figure 5 shows the resulting phonon transmission when the lattice relaxation is included and when it

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is ignored. All results in this paper are achieved with the nanodevice simulation tool NEMO5 [5].

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REFERENCES

[1] S. Datta, *Electronic Transport in Mesoscopic Systems*, Cambridge university press (1997)

[2] T. Boykin, et al. *Diagonal parameter shifts due to nearest-neighbor displacements in empirical tight-binding theory*, Phys. Rev. B 66, 125207 (2002)

[3] A. Paul, et al. *Modified Valence Force Field Approach for Phonon Dispersion : from Zinc-Blende Bulk to Nanowires*, J. of Comp. Elect. 9, Issue 3-4 (2010).

[4] S. Ahmed, et al. *Multimillion Atom Simulations with Nemo3D*, Encyclopedia of Complexity and Systems Science, pp 5745-5783 (2009).

[5] J. E. Fonseca, et al, *Efficient and realistic device modeling from atomic detail to the nanoscale*, J. of Comp Elect 12, 592 (2013).

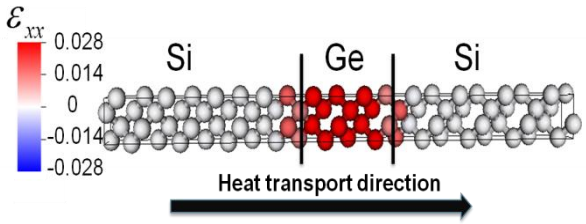

Fig. **1**. Strain component ε_xx of a 1.08nm thick Ge quantum well embedded in Si after relaxation.

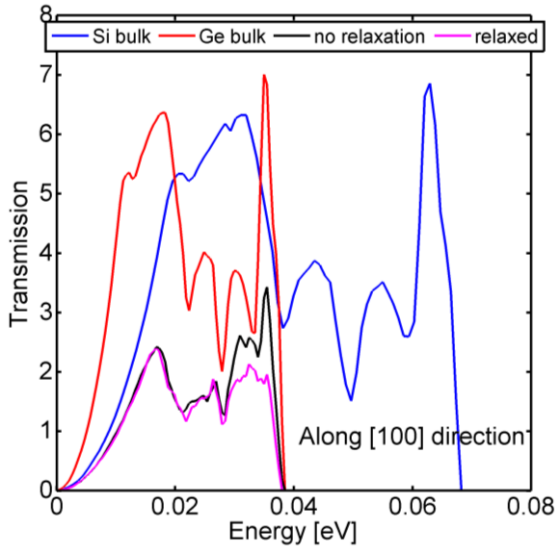

Fig. 2. Phonon transmission in pure Si, pure Ge and the Si/Ge/Si heterostructure of Fig. 1.

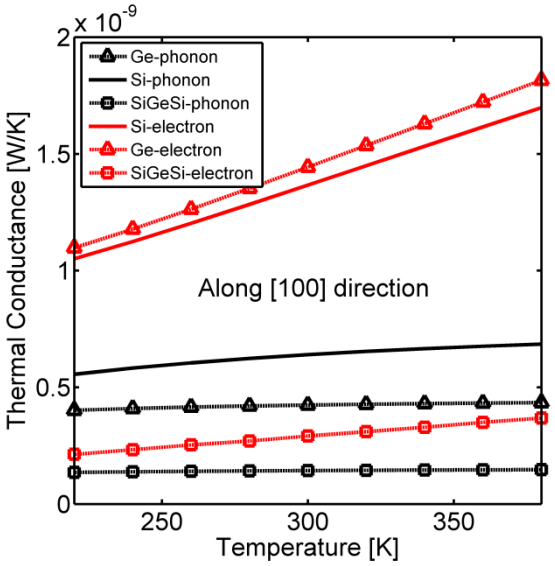

Fig. 3. Comparison of thermal conductance due to electrons and phonons of pure materials and the relaxed Si/Ge/Si heterostructure of Fig.1.

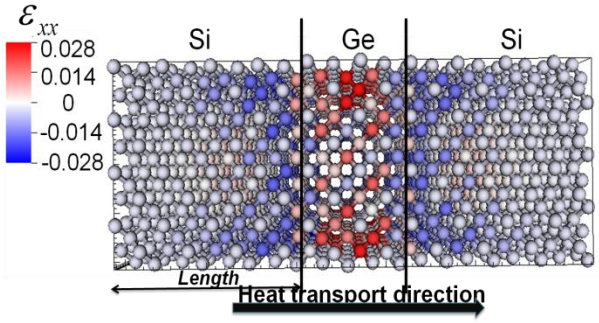

Fig. 4. Strain component ε_xx of 2.4 nm thick squared Si nanowire with a 1.2nm thick Ge layer after relaxation.

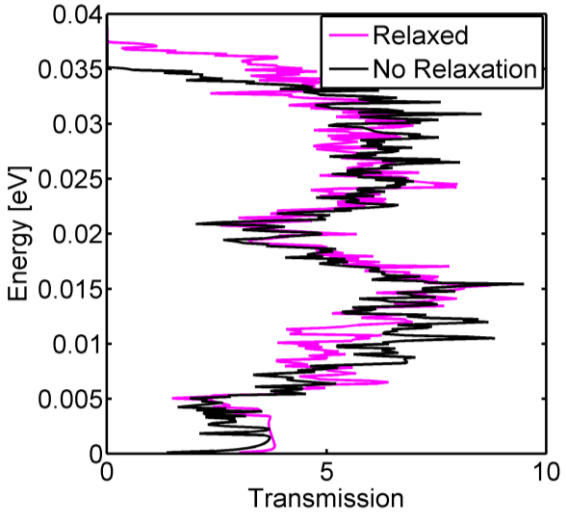

Fig. 5. Phonon transmission calculation of the nanowire in Fig. 4 with and without relaxation.