Mobilities and thermal conductivity from transport combined with molecular dynamics

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INTRODUCTION

At room temperature, electron-phonon (el-ph) scattering is typically the limiting factor for electron/hole mobilities. Also, anharmonic phonon-phonon (ph-ph) scattering is the governing scattering mechanism for phonons at room temperature, thus limiting the thermal conductivity. In this work, we combine Green's function based transmission calculations with molecular dynamics (MD) simulations in order to address both el-ph and ph-ph scattering. Preliminary results for silicon show good agreement between experiments and calculated phonon-limited electron- and hole mobilities and also between calculated and experimental phonon (lattice) thermal conductivities.

METHOD AND RESULTS

A general setup for our calculations is shown in Fig. 1. In a central region (MD) we allow the atoms to vibrate out of their equilibrium positions by performing MD simulations. For the MD and phonon transport simulations we use the semi-classical Tersoff potential as implemented in ATK[1]. For electron (hole) transport we describe the electronic hamiltonian with a $sp^3d^5s^*$ nearest neighbor tight-binding model, also available in ATK. We calculate electron- and phonon transmission functions using a standard Green's function method. Electronic transmission functions are all calculated a zero bias.

We wish to address bulk properties such as mobility and conductivity. In order to obtain such properties, we compute the energy- and temperature dependent scattering resistance[2] as

$$R_s(E,T) = \frac{1}{\mathcal{T}(E,T)} - \frac{1}{\mathcal{T}(E,T=0)} \qquad (1)$$

where $\mathcal{T}(E,T)$ is either the electron or phonon transmission function at energy E, and temperature T. By defining a resistivity as $\rho = R_s/L_0$, where L_0 is the length of the MD region, we can obtain bulk-like properties from ρ with proper integrations over energy with either the Fermi-Dirac function or the Bose-Einstein function for electron and phonon conductivities, respectively. An example of the linear dependence of R_s vs. L_0 is shown in Fig. 2.

Preliminary results for electron- and hole mobilities of bulk silicon are shown in Fig. 3, while Fig. 4 show the phonon thermal conductance of silicon vs. temperature. For both mobilities and thermal conductivities we obtain a rather close agreement with experimental results with difference within a factor of three.

CONCLUSION

We have presented a computationally very simple method for calculating el-ph and ph-ph scattering. We have evaluated the method by comparing calculated mobilities and thermal conductivities to experimental values, and found a generally good agreement.

ACKNOWLEDGMENT

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REFERENCES

[1] Atomistix ToolKit version 14.2, QuantumWise A/S (www.quantumwise.com).

[2] T. Markussen, R. Rurali, A.-P. Jauho, and M. Brandbyge, *Scaling Theory Put into Practice: First-Principles Modeling of Transport in Doped Silicon Nanowires*, Phys. Rev. Lett. **99**, 076803 (2007)

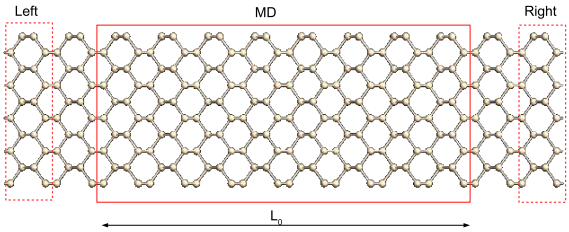

Fig. 1. Schematic setup of a calculation structure. Left and right semi-infinite electrodes are indicated within dashed boxed. In a central region of length L_0 we allow the atoms to be displaced away from their equilibrium positions, by performing MD simulations.

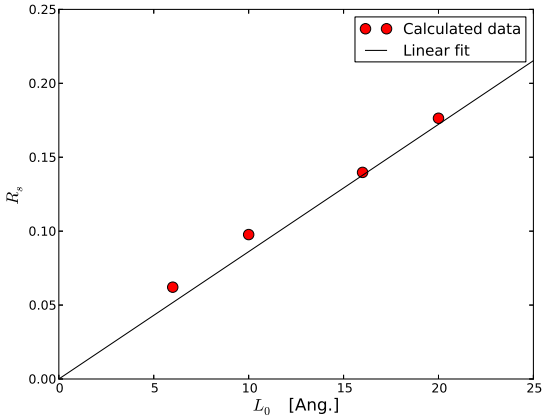

Fig. 2. Phonon scattering resistance vs. length of MD region (L_0) calculated at phonon energy $E_{ph} = 20\,\text{meV}$ and temperature 300 K.

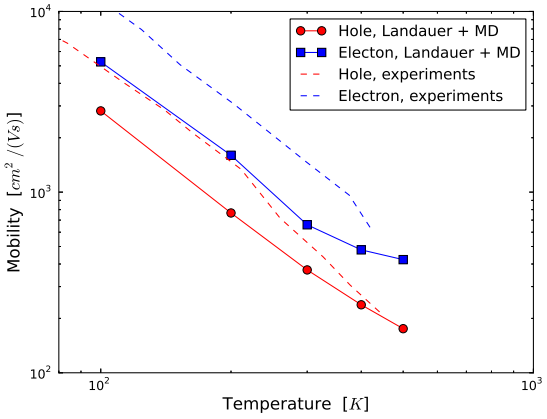

Fig. 3. Silicon hole (red) and electron (blue) mobilities vs. temperature. Calculated values are shown with symbols and solid lines, while experimental values for low doped silicon are shown as dashed lines.

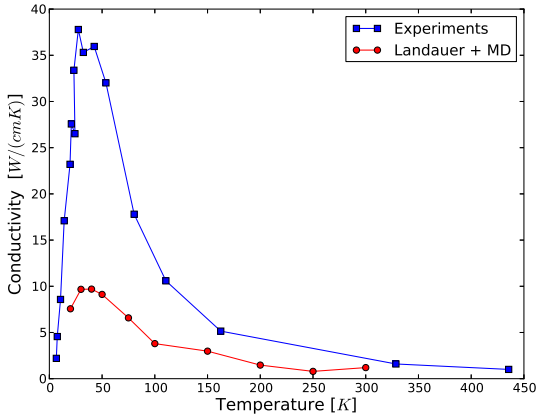

Fig. 4. Silicon thermal conductivity vs. temperature. Experimental values are shown as blue squares, while the calculated values are shown as red circles. Both calculated and experimental curves peaks around a temperature of 50 K. Around room temperature, the calculated values are within a factor of two of the experimental results.