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Molecular dynamics simulations supporting the development of a continuum model of heat transport in nanowires

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Extended Abstract

1. BACKGROUND

To save computational resources, calculation of thermal transport in TCAD tools dedicated to electron devices is usually based on continuum approaches. For nanoscaled devices, proper extensions of Fourier's law have to be implemented to reproduce effects arising from phonon confinement and interface scattering. To provide reliable data for the development of such model extensions, a suitable methodology for Molecular Dynamics (MD) simulations has been developed. It is based on an innovative combination of heat sources and Langevin thermostats applied to silicon nanorods with silicon dioxide caps that allows a direct validation on the basis of previous work as well as a direct comparison to continuum simulations based on equivalent boundary conditions.

2. METHODOLOGY

We consider axial heat transfer along Si nanowires heated uniformly with 15eV/ps through end lids coated by amorphous SiO_2 layers as shown in Fig.1. This structure design provides conditions for axial heat transfer including heat transport through the Si/SiO_2 interface. Exploiting the freely available simulation tool LAMMPS [1], stable version (3 Mar 2020), Non-Equilibrium Molecular Dynamics (NEMD) simulations were performed using Tersoff potentials. The atomic structure of the amorphous silicon dioxide material was simulated by a heating of crystalline SiO_2 above the melting point, followed by a rapid cooling. Periodic boundary conditions were set at the boundaries of the MD simulation box, indicated by black lines in Fig.1. In our previous work [2] similar structures with a heat source in the middle and heat sinks at the periphery have been validated already against literature data. Unfortunately, such a set-up, which is rather common in MD simulations, leads to numerical problems and ill-defined solutions in continuum approaches. To bridge MD to continuum simulations, we consider here in addition a NEMD set-up in which Langevin thermostats are applied in the outermost 4 Å of the SiO_2 boundary regions to establish there the lowest temperatures obtained by the first NEMD model. This set-up corresponds to Dirichlet boundary conditions imposed at the external SiO_2 boundary in the continuum model. For both NEMD approaches, steady state has established within the simulation time of 2 ns. In the continuum model taking into consideration phonon transport corrections, separate temperature fields (e.g. T_1 and T_2) in the material bulk regions are ruled by a Fourier law-like heat equation with the bulk conductivity values (e.g. k_1 and k_2). Standard continuity conditions (T_1=T_2) at the interface between different materials are replaced by jump conditions (see Eq. 5 of Ref. [3]), ruled by the local functional $(k_1/\lambda_1 + k_2/\lambda_2)|_\Gamma$ at the Γ interface location, where λ_i is the average phonon mean free path in the i-material. A thermal conductivity value of 2.1 W/K/m was taken for the bulk amorphous SiO_2 from MD simulations reported in the literature [4], while the (temperature-dependent) experimental value was used for bulk Si [3]. Accurate discontinuous Galerkin solutions for the steady state have been obtained and the present setting can be used for large scale modeling of thermal transport in electronic devices. We notice that when fixing the conductivity values the interface discontinuity depends on the estimates of λ_i.

3. RESULTS

Figures 2-4 show that the continuum model and two different NEMD models provide similar temperature distributions along uniformly heated Si nanowires when heat is released through the nanowire end lids coated by amorphous SiO_2 layers with different thicknesses.

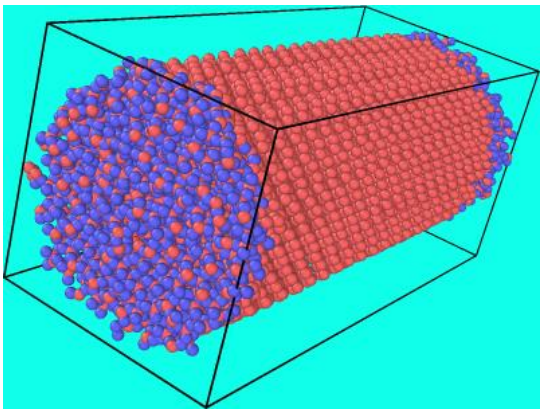

Fig. 1. Atomic arrangement consisting of 13748 atoms for the MD modelling of a 10-nm-long cylindrical Si nanowire with a diameter of 5.2 nm and with end lids coated by 1-nm-thick amorphous SiO_2 layers. The figure was created by using OVITO [5].

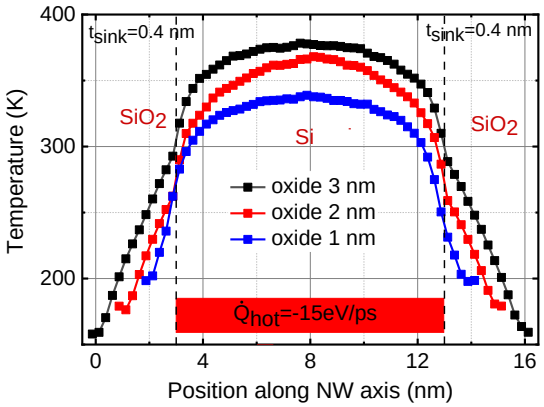

Fig. 2. Temperature distribution along the axis of the cylindrical nanowire obtained in the first NEMD model. Two heat sinks with powers of 7.5 eV/ps each are set in the a-SiO_2 layers on the Si nanowire tips.

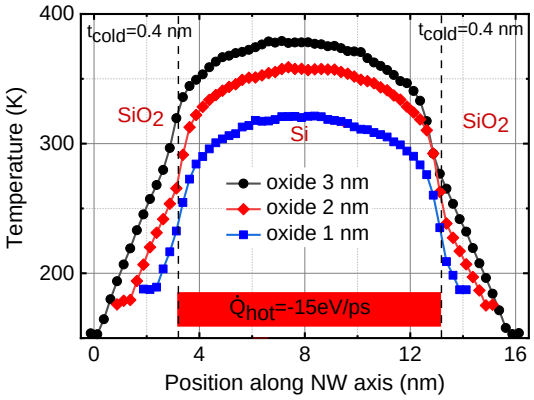

Fig. 3. Temperature distribution along the axis of the cylindrical nanowire obtained in the second NEMD model. The lowest temperatures in the thermostat-controlled regions are 187, 175, and 153 K for the a-SiO_2 layers with thicknesses of 1, 2, and 3 nm, respectively.

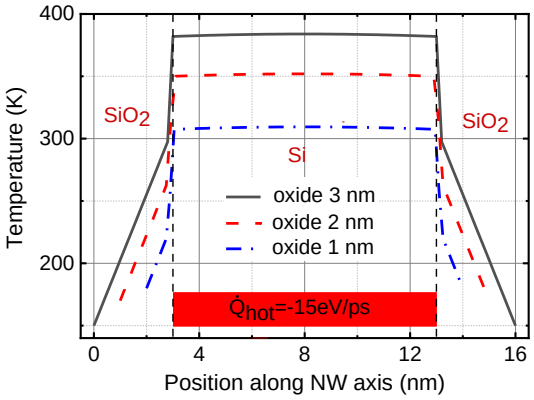

Fig. 4. Temperature distribution along the axis of the cylindrical Si nanowires with 1-, 2-, and 3-nm-thick amorphous SiO_2 layers on the nanowire tips obtained in the continuum model. $\lambda_{Si} = 59.6\ nm$ and λ_{SiO_2} =30.2 nm in this case.

4. CONCLUSIONS

We have developed a set-up of thermal boundary conditions that can be used equivalently in both molecular dynamics and continuum simulations. With its help, it will be possible to provide relevant data for the development and calibration of TCAD continuum models suitable for nanoscaled electron devices.

5. REFERENCES

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