MODELING OF THERMAL TRANSPORT IN ELECTRONIC NANO-DEVICES USING METHODS OF MOLECULAR DYNAMICS

V.I. Belko, belko@bsu.by

Belarusian State University, Minsk, Belarus

1. INTRODUCTION

Numerical modeling of technological processes and devices has become an important economical factor in microelectronics. Now, a very important transition to nano-scaled elements in semiconductor microelectronics is in progress. Extremely high current densities and a high device package density result in a significant heating of separate devices and of the whole integrated circuits. Therefore the problem of the heat management in integrated circuits becomes one of the major challenges for nano-scaled electronics. Conventional methods of the simulation of the thermal transport based on the Fourier equation are insufficient for the description of the thermal transport in device structures that contain small nano-metric features. The reason for this is that the main heat transport mechanism in semiconductors and insulators is the phonon assisted heat transport, and the mean free path of the phonons has a wide spectrum ranging from about 10 nm to millimeters. Therefore for small device features and also for small hot spots that are comparable in size with the mean free path of the phonons participating in thermal transport deviations from the conventional diffusion-like thermal transport is expected.

Here the method of molecular dynamics will be applied for the simulation of the thermal effects typical for nano-scaled electronic devices. The advantage of the method is in its universal applicability. We do not need to know in advance the properties of certain phonon modes. The phonons appear in the simulations in a natural way and all reflections and scattering effects are accounted for without any special measures. It should be mentioned that in the method of molecular dynamics we have to define the atomic structure of the whole simulation sample, and we have to know the interatomic potentials for the materials considered. The interatomic potentials in silicon are well known. There are also models of the interatomic potentials published for silicon dioxide.

There are three principal techniques used to evaluate the thermal conductivity via molecular dynamic simulations [1] (i) the equilibrium approach based on the Green-Kubo method (ii) heat source and sink, also called direct method, non-equilibrium molecular dynamics (NEMD) based on the creation of temperature gradient, (iii) and the homogeneous NEMD, where a heat flux is induced, however, without a temperature gradient thus allowing to use periodic boundary conditions in a similar manner as in the equilibrium approach.

In this paper the direct NEMD method was applied, where a heat flux is induced and the resulting temperature gradient was measured. Specifically, we applied the open-source program LAMMPS [2]. This program allows a parallel computing on several CPUs using the Message Passing Interface paradigm of computing distribution.

2. RESULTS AND DISCUSSION

Let us consider a model sample of a silicon crystal in the form of a rectangular parallelepiped. The parallelepiped is elongated in the direction x, along which an artificially formed thermal gradient will be established. In the area near the right end of parallelepiped an incoming heat flux will be generated (by means of increasing particle velocity in accordance with a desired quantity of flow). Similarly, at the left end the heat sink will be formed. The system is first allowed to reach a steady state at given temperature (300 K). Then, after a relatively long simulations with fixed heat flow a temperature gradient will be formed in the sample. As a result, we can estimate the thermal conductivity based on the Fourier law. The results obtained for the temperature of 300 K, and various combinations of the sample size and boundary conditions are shown in table 1.

Table 1. The calculated values of the thermal conductivity

Potential	Sample size, the number of unit cells	Boundary conditions on *x,y,z*	Sample description	Thermal conductivity, W/m·K
Tersoff	14x8x8	FPP	nanolayer	15.6
Tersoff	28x8x8	FPP	nanolayer	39.2
SW	14x4x4	FFF	nanowire	4.7
SW	20x4x4	PPP	bulk crystal	6.2

Thus, the calculations for the case of a thin silicon layer (7.6 nm and 15.2 nm, respectively) show an increase in thermal conductivity depending on the thickness of the layer. The obtained values are significantly lower than the experimentally measured in solid silicon. The result for the nanowire (sample with free boundary conditions in all three dimentions) is comparable to the result of the paper [3], where the relaxation time for the formation of a temperature gradient was much longer and the obtained value of the thermal conductivity is of the order of 1 W/m·K. Finally, the value of the coefficient for a sample with periodic boundary conditions in all directions corresponds to the result of 5 W / m · K from [4], where the relaxation time was also significantly longer.

Let us note also that LAMMPS package allowed use the acceleration due to parallel execution on multiprocessor systems in all simulations. Moreover, the control commands allow to specify the incoming and outgoing heat fluxes without code modification. However, it is relatively difficult to choose the simulation parameters so as to produce a temperature gradient and without destroying the dynamics of the system.

References

1. Termentzidis, K. Nonequilibrium molecular dynamics simulation of the in-plane thermal conductivity of superlattices with rough interfaces / K. Termentzidis, P. Chantrenne, P. Keblinski // Physical Review. 2009. Vol.79B. P.214307.
2. LAMMPS Molecular Dynamics Simulator // [Electronic resource]. – January, 2009. – Mode of access: http://lammps.sandia.gov/. – Date of access: 01.05.2014.
3. Yang, X. Anomalous heat conduction behavior in thin finite-size silicon nanowires / X. Yang, A. To, R. Tian // Nanotechnology. 2010. Vol.21. P.155704.
4. Srinivasan, S. On parallel NEMD simulations of heat conduction in heterogeneous materials with three-body potentials: Si/Ge superlattice / S. Srinivasan, R.S. Miller // Numerical Heat Transfer. 2007. Vol. B52. P. 2971998.