STUDY OF PHONON HEAT TRANSFER IN METALLIC SOLIDS FROM MOLECULAR DYNAMICS SIMULATIONS

Patrice CHANTRENNE, Martin RAYNAUD, Dominique BAILLIS
Thermal Center of Lyon UMR CNRS 5008, INSA, Bât. Sadi Carnot, 20, Av. Albert Einstein
69621 Villeurbanne Cedex, France

To describe the thermal behaviour of nanostructured materials and nanoelectronic devices, new properties and models have to be determined at the atomic scale. Recent experimental techniques such as near field microscopy[1-2] allow to investigate heat transfer at small scales, but, the spatial resolution is still greater than 50 to 100 nm. This remains too large when the typical length of interest is a few nm. Moreover, at this scale, the sensor may have a significant influence on the temperature or the property to be measured. Numerical simulation is then the solution to study the matter at the atomic scale and to predict the thermophysical properties of solids.

Molecular dynamics allows to simulate the material behaviour at the atomic scale[3-4]. It requires the knowledge of potentials that describe the interaction between atoms. As Si and Ge are semi conductors widely used for electronic components, accurate potential were determined for these materials[5]. Recently, heat transfer in nanostrutures made of Si or Ge has been studied and heat conductivity has been calculated[6-7].

Metallic solids are also widely studied using molecular dynamics. Due to their cristallographic structure, potentials[8-9] are quite different than those used for semi conductors and leads to a more efficient implementation of the molecular dynamics. In metallic solids, the main contribution to heat transfer resistance is due to electron-phonon interactions. For very pure metals, theoretical models to calculate thermal conductivity do not even take into account phonon-phonon contribution to heat transfer resistance[10-13]. For temperature greater than Debye temperature, the heat transfer resistance due to phonon-phonon interaction may increase while heat transfer resistance due to phonon-electron interaction should remain constant. It is interesting to note that the thermal conductivity decreases more or less rapidly, depending on metallic material, when temperature increases. It can be interpreted as an effect of the phonon-phonon interaction which becomes non negligible for poorly conducting metals and alloys.

The Wiedemann-Franz[11] states that for metals, the ratio of electronic thermal conductivity, λ_e, to the electrical conductivity, σ, is proportional to the temperature :

$$\lambda_e = \sigma L T$$

with $L = 2.45\,10^{-8}$ $W\Omega/K^2$, the Lorenz number which should not depend on the nature of the metal. So, if the total thermal conductivity and the electrical conductivity are known, it should be possible to calculate the electronic thermal conductivity and then the phonon thermal conductivity. Using values of reference from thermophysical properties tables[10], negative values can be found for the phonon-phonon thermal conductivity. This shows either a lack of accuracy of the data or the unreliability of the model. Usually, as the Wiedemann-Franz law comes from a simplify model and approximations, it is admitted that the Lorenz number may vary for each metal. It is then calculated from experimental value of thermal and electrical conductivity, assuming that the phonon-phonon interaction are negligible[11-12].

Molecular dynamics is used to study phonon-phonon interaction heat transfer resistance in metallic solids in order to evaluate their importance towards the total heat transfer resistance. Calculation are made for aluminium which is a fairly good heat transfer conductor.

The field of heat transfer at atomic scale includes temperature, energy, heat flux and thermal conductivity calculation. The definition and calculation methods are reviewed. The method proposed by Kotake and Wakuri[14] based on Non Equilibrium Molecular Dynamics, has been adapted to decrease the computational time and simplify its implementation. It leads to the calculation of heat flux between two blocs at different imposed temperatures separated by an intermediate bloc (Figure 1) in which the temperature profile can also be determined. The spatial periodic boundary conditions are used in the z direction so that heat flux and temperature gradient are calculated in two independent blocs simultaneously.

Aluminium is an fcc metal with a lattice parameter a_0 equal to 0.4032 nm. The system geometry is shown on figure 1. The orientation of the crystal is [100], [010] and [001] and the dimensions are $n_x a_0$, $n_y a_0$ and $n_z a_0$ in the x, y and z directions respectively. This crystal is placed in a periodic box which dimensions in the x, y and z directions are equal to $n_x a_0$, $n_y a_0$ and $n_z a_0$ to simulate an infinite solid in the x and y directions. Temperature gradient and heat flux are calculated for different thickness of the intermediate blocs. There are two possible approaches to explain the temperature gradient :

- in the first one, an attempt is made to calculate the thermal conductivity, using the linear part of the gradient. The non linear parts are considered as transition regions due to the interface thermal resistance between the thermostats and the intermediate blocs. It is shown that, in our case, the thermal conductivity and thermal resistance vary with the thickness of the intermediate blocs.
- in the second one, it is shown that the non dimensional temperature gradient exhibit the same kind of profile than the one given by radiative heat transfer. This means that phonon transport is mainly ballistic. Using a code solving the radiative transfer equation in a semi-transparent media, based on the discrete ordinate method[15], the equivalent radiative properties are determined.

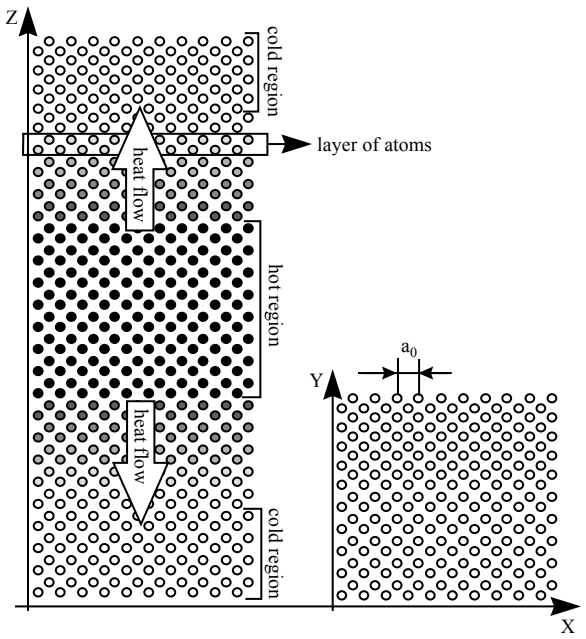

Figure 1 : Geometry of the system. The atoms are placed in a box which is repeated boundary conditions are used in the three directions.

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