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MOLECULAR DYNAMIC SIMULATION OF NANOSCALE HEAT TRANSFER

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Recent developments of industrial applications in the field of microelectronics, microheat exchangers, laser systems, bioengineering, analytical chemistry have induced scientific studies dealing with microscopic behaviour of phenomena like heat transfer, or microfluidics, at very tiny scales. The results have shown that the physical mechanisms of thermal transport in extremely small length and extremely short time differ sensibly from those in the macro-scale world.

Whereas all the different modes of heat transfer are to be reconsidered when decreasing the space scales, radiation, convection, boiling phenomena in micro channels, for instance, this paper will deal essentially with heat conduction in solids at molecular level.

After a quick survey of the basis of macroscopic laws for heat transfer and of the classical method of modelling, some example of industrial applications will be commented upon: this will allow to demonstrate the specificity of the emergence of new heat transfer problems linked to size effects, like in electronics superlattices, or in silica aerogels which provides efficient superinsulation. One of the difficulties came from the fact that the first experimental results showed a new behaviour of the thermal conductivity, namely, its decrease while decreasing for instance the thickness of the sample. Some basic questions concerning heat transfer, when starting from micron, towards nanometers scale will be discussed: which theoretical tools, which modelling tools, and which measurements techniques can be used?

We shall focus on modelling heat transfer in solids with the Molecular Dynamic, which will be demonstrated to be an efficient technique to handle heat transfer at atomic level, and provides then a gateway to submicron heat transfer in micro/nanosystems. One of our objectives is the computation of the thermal conductivity of crystalline solids.

Starting from the analysis of the microscopic forces responsible for interaction between atoms, the expression of these forces can be obtained from a potential which will be considered as data for the analysis of the heat transfer process, which means that we rely on the expertise of specialists of physics to provide us these potentials. This is an important point to observe that, according to the nature of the structure of the solid, the potential will be more or less complex. In any case, the forces will be obtained by a derivation process of the potential.

According to the Newton law, the mechanical balance of a given atom will be described by a second-order ordinary differential equation, which means that a set of atoms will be described by a set of coupled non-linear differential equations to be solved. The solution of this set of equations provides the positions, the velocities and the acceleration of the atoms. A first step is then accomplished, which is the microscopic description of the mechanical analysis of the system.

A further step is to extract from these microscopic mechanical information, the thermal variables: temperature, energy, heat flux. The total energy is readily available, from the expression of its kinetic and potential components. The most interesting variable to get is then the heat flux, which gathers the convected energy and the work of the interaction forces, and a particular treatment will lead to the autocorrelation function of this heat flux. An intuitive idea is that this autocorrelation function of the heat flux contains information about the way heat is locally transported by the atoms: the conductivity can effectively be deduced from this auto correlation function through the Green Kubo formula. This is the basic procedure that we first applied to the computation of the thermal conductivity of argon.

Because of a relatively modest performance we also developed an improved version which is known as the non equilibrium molecular dynamic.

Three typical examples will be presented, all dealing with the computation of the thermal conductivity.

The first one concerns argon, for which the potential is the classical Lennard-Jones one, implying the description of the attractive and repulsive forces at the atomic level. The agreement with experimental data is rather fair, for temperatures for which we can neglect quantum effects.

The second example is the case of silicon. It is a bit more complex, because the potential has to translate the covalent characteristic of the chemical bound. We shall retrieve the well- known dependence law Conductivity vs. Temperature in 1/T.

The third one will deal with silica and more particularly with alpha-quartz, the potential of which is still more complicated: it must describe the position of Si and O atoms and the short and long range forces involved, which implies rather long calculations for this, but the same global procedure can be used. We still retrieve the experimental data for this anisotropic material.

The last example will present results we have gained on the heat transfer in nanoparticles of silica. The configuration is different from the previous ones: instead of a perfect crystal, the atoms are aggregated in two particles, the size of which is nanometric; the mean distance between the particles is also nanometric, and we simulated a set of two such nanoparticles. The main question is here how the heat is transferred from one nanoparticle to the other.

As a matter of conclusion, we have here an example of a scientific problem which has been pushed by the emergence of nanotechnologies (microelectronics, oproélectronics) and for which a need appeared to explain what happened to heat transfer when dealing with such small space scales.

The work we present concerns rather the methodology of computation, but we have used it in the case of thin films or nanowires, for which we have shown a strong dependence of the conductivity relatively to the geometrical dimension. Clearly, heat transfer always affects at atomic level, but this has large consequences when the size of the object becomes of the order of magnitude of the carrier of heat, and this implies, for instance, a big decrease of conductivity in very tiny objects.