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Thermal Transport at the Nanoscale



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Understanding and controlling the thermal and electronic properties of nanostructured materials and devices are of great interest in a large scope of contexts and applications: biology and medicine, aerospace, communications, computers, electronics and energy applications. The behavior and reliability of these devices strongly depend on the way the system releases heat, as excessive temperatures or temperature gradients result in their failure. A predictive theory for the thermal conductivity assessment is essential for the design of new materials. This is particularly true for efficient thermoelectric devices and to control the heat dissipation in micro and nanoelectronics. The correlation between grain boundaries, interfaces and surfaces and the thermal transport properties is a key point to design materials with tailored properties and systems with a controlled behavior. During this seminar, all these issues will be addressed and a number of examples of thermal transport properties obtained by

Molecular Dynamics (MD) simulations will be given (nanowires, superlattices). The common feature of these systems is the small ratio between their characteristic system size and the phonon mean free path, which leads to a ballistic heat transport.

Furthermore, when the density of interfaces gets large, the energy transport properties of the materials cannot longer be described solely by the thermal conductivities of the constituents of the material, but depend also on the thermal boundary resistance which measures the transmission of phonons across an interface. In this context, molecular dynamics was proven to be a very useful technique to study heat transport in nanostructured materials. The main reasons are; the length scale probed by the method is in the nanometer range, and it does not make any assumption on the phonons dynamics except their classical nature.

Το προφίλ του ομιλητή



Konstantinos TERMENTZIDIS is a CNRS researcher and he works at the *LEMTA laboratory*, at the University of Lorraine, France since 2012. He started his studies at the *Aristotle University of Thessaloniki* (Physics Departement and Master Material's Physics and Technology), and he obtained his PhD at the *University of Vienna*, at the Computational Material Science group, under the supervision of Professor Jurgen HAFNER. He worked as a postdoc fellow at *INSA of Lyon* and at the *Ecole Centrale Paris*. His main scientific interest is the theoretical and computational nanoscale heat transport. During, the last 6 years he is studying the phonon transport at nanowires and superlattices with molecular dynamics, with an important publication production in the domain. The nanoscale heat transfer is a crucial issue for a large scope of contexts and applications as biology, medicine, aerospace, communications, electronics and energy. The behavior, reliability, life and cost of these devices depend on the way the system releases heat. As experimental studies are not always available or suitable at this scale, dedicated models and simulations tools are necessary. Termentzidis with his work elucidated the interaction of phonons with interfaces and surfaces at the nanoscale, a key point to design materials with tailored properties and systems with controlled behavior.