Nanoscale heat flow predictions

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Physicists are now designing novel materials with physical properties tailored to meet specific energy consumption needs. Before these so-called materials-by-design can be applied, it is essential to understand their characteristics, such as heat flow. Now, a team of Italian physicists has developed a predictive theoretical model for heat flux in these materials, using atom-scale calculations.

The research, carried out by Claudio Melis and colleagues from the University of Cagliary, Italy, is published in the *European Physical Journal B*. Their findings could have implications for optimising the thermal budget of nanoelectronic devices—which means they could help dissipate the total amount of thermal energy generated by electron currents—or in the production of energy through thermoelectric effects in novel nanomaterials.

The authors relied on large-scale molecular dynamics simulations to investigate nanoscale thermal transport and determine the corresponding physical characteristics, which determine thermal conductivity. Traditional atomistic calculation methods involve a heavy computational workload, which sometimes prevents their application to systems large enough to model the experimental structural complexity of real samples.

Instead, Melis and colleagues adopted a method called approach equilibrium molecular dynamics (AEMD), which is robust and suitable for representing large systems. Thus, it can use simulations to deliver trustworthy predictions on thermal transport. The authors investigated the extent to which the reliability of the AEMD method results is

affected by any implementation issues.

In addition, they applied the method to thermal transport in nanostructured silicon, a system of current interest with high potential impact on thermoelectric technology, using simulations of unprecedented size. Ultimately, the model could be applied to semiconductors used as high-efficiency thermoelectrics, and to graphene nanoribbons used as heat sinks for so-called ultra large scale integration devices, such as computer microprocessors.

More information: C. Melis, R. Dettori, S. Vandermeulen and L. Colombo (2014), Calculating thermal conductivity in a transient conduction regime: theory and implementation, *European Physical Journal B*, DOI: 10.1140/epjb/e2014-50119-0

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