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Thermal Conduction and Thermoelectics in Nanoscale

Professor Nuo YANG

School of Energy and Power Engineering,
Huazhong University of Science and Technology (HUST), Wuhan, China

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In the past decades, rapid developments in synthesis and processing of nanoscale materials have created a great demand for understanding of thermal transport in low dimensional nanomaterials.

The polymers with high thermal conductivity have a widely application in heat dissipation. Recently, we found new ways to enhance the thermal conductivity of polyethylene. Different from traditional methods, such as random doping, we find that the aligned carbon nanotube-polyethylene composites [Sci. Rep. 5, 16543 (2015)] and paved crosswise laminate polyethylene [arXiv:1605.01540] have high thermal conductivities by molecular dynamics simulations.

On the other hand, thermoelectric materials can generate electric power directly from the heat, which can be used in harvesting waste heat. The nanostructured thermoelectric material are studied widely on reducing the thermal conductivity. However, it is still far from having a recipe for nanoscale thermoelectric materials with a higher figure of merit (zT). Recently, we found a new idea to enhance the zT that is to increase the power factor of the structure with low thermal conductivity [Nano Lett 15, 5229 (2015)]. By calculations, we showed that the nanostructured bis-dithienothiophene molecular crystal is a candidate for such an approach. We obtained a maximum room-temperature zT of 1.48 at optimal doping.

The concept of functionally graded material (FGM), a composite of two or more phases, was proposed in 1984 as a means of preparing thermal barrier materials. Naturally, the thermal conductivity is a constant for the most nanostructures, such as carbon nanotube and graphene, which means that the they are homogeneous. However, recently, we found a graded (non-homogeneous) thermal conductivity along the radius direction in the graphene disk [Sci. Rep. 5, 14878 (2015)] and carbon nanocones [arXiv:1605.01471] by both numerically and analytically.

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本件連絡先: 東京大学大学院工学系研究科機械工学専攻 准教授 塩見 淳一郎
GMSIプログラム事務局 E-mail: office@gmsi.t.u-tokyo.ac.jp Phone: 03-5841-0696