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COMPUTATIONAL NANOMECHANICS AND NANOSCALE THERMAL TRANSPORT

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HAIFEI ZHAN[*], HENGAN WU[†], GANG ZHANG[+], YUANTONG GU[*]

[*]Queensland University of Technology
2 George ST, Brisbane QLD 4000, Australia
zhan.haifei@qut.edu.au, https://staff.qut.edu.au/staff/zhan.haifei

[†]University of Science and Technology of China
Hefei, Anhui 230027, China

[+]Institute of High Performance Computing
1 Fusionopolis Way, Singapore 138632, Singapore

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ABSTRACT

The advancing of nanotechnology has enabled the fabrication of high-performance functional materials and the continuing miniaturization of mechanical devices or systems. To facilitate the manufacturing and applications of nanoscale materials, it is vital to understand their mechanical properties. There are have been extensive experimental, theoretical, and computational efforts at atomistic scale to understand the mechanical behaviours of nanomaterials. Particularly, for the novel structures with extreme small dimensions like the ultra-thin diamond nanothread [1], the atomic simulations have provided useful guidelines for the experimental study.

Besides the mechanical properties, the thermal transport of the nanomaterials is another fundamental characteristic that determine their usages [2]. Depending on the application, materials are required to have a high thermal conductivity or a strongly suppressed thermal conductivity. For instance, for energy saving in both residential and commercial buildings and thermoelectric devices, there has been a continuing search for high performance materials with a low thermal conductivity. In comparison, a high thermal conductivity is required for the electronic packing to enable efficient heat removal and transfer.

The diversity of low dimensional nanomaterials has provided a great potential to construct novel nanostructures with required mechanical and thermal performance. This mini-symposium intends to bring the recent progress on atomistic simulations for the mechanical and thermal transport properties of nanomaterials, which serve as effective tools to guide experiments or predict novel nanomaterials.

REFERENCES

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