Tech Science Press

ICCES, 2024, vol.32, no.3
DOI: 10.32604/icces.2024.012552

PROCEEDINGS

Deep-Potential Enabled Multiscale Simulation of Interfacial Thermal Transport in Boron Arsenide Heterostructures

Jing Wu[1], E Zhou[1], An Huang[1], Hongbin Zhang[2], Ming Hu[3] and Guangzhao Qin[1,*]

[1]State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body, College of Mechanical, Hunan University, Changsha, 410082, China

[2]Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, 64289, Germany

[3]Department of Mechanical Engineering, University of South Carolina, Columbia, SC 29208, USA

[*]Corresponding Author: Guangzhao Qin. Email: gzqin@hnu.edu.cn

ABSTRACT

High thermal conductivity substrate plays a significant role for efficient heat dissipation of electronic devices, and it is urgent to optimize the interfacial thermal resistance. As a novel material with ultra-high thermal conductivity second only to diamond, boron arsenide (BAs) shows promising applications in electronics cooling [1,2]. By adopting multi-scale simulation method driven by machine learning potential, we systematically study the thermal transport properties of boron arsenide, and further investigate the interfacial thermal transport in the GaN-BAs heterostructures. Ultrahigh interfacial thermal conductance of 260 MW $m^{-2}K^{-1}$ is achieved, which agrees well with experimental measurements, and the fundamental mechanism is found lying in the well-matched lattice vibrations of BAs and GaN [1,3,4]. Moreover, the competition between grain size and boundary resistance was revealed with size increasing from 1 nm to 100 μm. The results are expected to lay theoretical foundation for the applications of BAs in advanced thermal management of electronic devices [5].

KEYWORDS

Machine learning; multiscale simulation; boron arsenide; interfacial thermal transport

Acknowledgement: The numerical calculations in this paper have been done on the supercomputing system of the National Supercomputing Center in Changsha.

Funding Statement: We acknowledge the support of the National Natural Science Foundation of China (Grant Nos. 52006057), National Key R&D Program of China (2023YFB2408100), the Fundamental Research Funds for the Central Universities (Grant No. 531119200237), the Natural Science Foundation of Chongqing, China (No. CSTB2022NSCQ-MSX0332), and the State Key Laboratory of Advanced Design and Manufacturing for Vehicle Body at Hunan University (Grant No. 52175013), and the Outstanding Youth Project (23B0024) of Hunan Provincial Department of Education.

Conflicts of Interest: The authors declare that they have no conflicts of interest to report regarding the present study.

References

1. Wu, J., Zhou, E., Huang, A., Zhang, H. B., Hu, M., Qin, G. Z. (2024). Deep-potential enabled multiscale simulation of gallium nitride devices on boron arsenide cooling substrates. *Nature Communications, 15,* 2540.

2. Qin, G. Z., Xu, J. H., Wang, H. M., Qin, Z. Z., Hu, M. (2023). Activated lone-pair electrons lead to low lattice thermal conductivity: a case study of boron arsenide. *The Journal of Physical Chemistry Letters, 14,* 139-147.
3. Yu, L. F., Xu, J. Y., Shen, C., Zhou, E., Wu, J., Zhang, H. B., Zheng, X., Wang, H. M., Qin, G. Z. (2023). Realizing ultra-low thermal conductivity by strong synergy of asymmetric geometry and electronic structure in boron nitride and arsenide. *Rare Metals, 42,* 210-221.
4. Qin, G. Z., Qin, Z. Z., Wang, H. M., Hu, M. (2018). Lone-pair electrons induced anomalous enhancement of thermal transport in strained planar two-dimensional materials. *Nano Energy, 50,* 425-430.
5. Wu, J., Huang, A., Xie, H. P., Wei, D. H., Li, A., Peng, B., Wang, H. M., Qin, Z. Z., Liu, T. -H., Qin, G. Z. (2023). Multi-scale Simulation of Mechanical and Thermal Transport Properties of Materials Based on Machine Learning Potential. *Journal of the Chinese Ceramic Society, 51,* 531-543.