Substrate influence on the thermal rectification of hBN-C heterostructures

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Abstract

Here, we study the influence of substrate on the thermal transport properties of hBN-C nanostructures with strong structural asymmetries (see Fig. 1) by using non-equilibrium molecular dynamics (NEMD) simulations [1]. We show that thermal rectification ratios of up to 20 % can be achieved in dependence of the asymmetry degree of the free-standing ribbons. Moreover, by depositing the nanoribbons on different substrates, the heat flux is improved but the thermal rectification is reduced (see Fig. 2). We have considered two different geometrical shapes for hBN-C thermal rectifiers: T-shaped and triangular. To quantify the degree of structural asymmetry of the nanoribbons, the dimensionless quantity $W_{LR} = W_{Left}/W_{Right}$ is introduced [2]. Here, W_{Left} and W_{Right} are the widths of the left and right ends of the nanoribbons, respectively, and the case $W_{LR} = 1.0$ corresponds to a fully symmetric rectangular ribbon. We remark that nanostructures as those investigated here may be already accessible to state of the art experimental approaches [3]. Thus, we expect our results to shed light on the potential of 2D materials for the engineering of highly efficient thermal devices.

References

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[3] Y. Gao, Y. Zhang, P. Chen, Y. Li, M. Liu, T. Gao, D. Ma, Y. Chen, Z. Cheng, X. Qiu, W. Duan, Z. Liu, Nano Lett., 13 (2013) 3439.

Figures

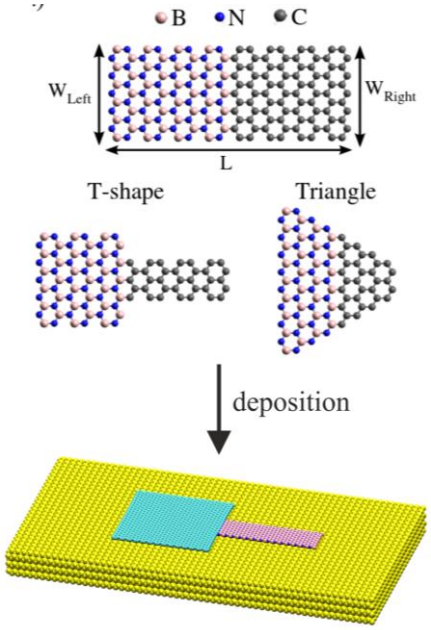

Figure 1: Asymmetrical geometrical shapes selected for our hBN-C nanoribbons. Scheme of nanoribbons deposited on a substrate.

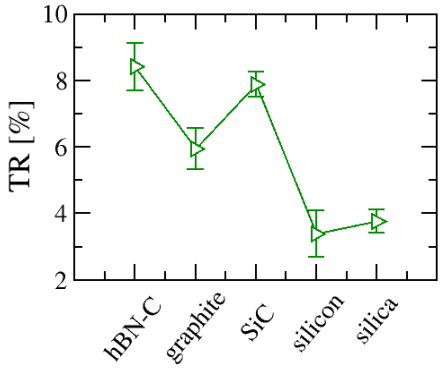

Figure 2: Variation of thermal rectification (TR) with the substrate for T-shaped hBN-C nanoribbons with $W_{LR} = 1.0$.