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Thermal conductivity of random polycrystalline BC_3 nanosheets: A step towards realistic simulation of 2D structures

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Abstract

Boron carbide nanosheets (BC_3NSs) are semiconductors possessing non-zero bandgap. Nevertheless, there is no estimation of their thermal conductivity for practical circumstances, mainly because of difficulties in simulation of random polycrystalline structures. In the real physics world, BC_3NS with perfect monocrystalline is rare, for the nature produces structures with disordered grain regions. Therefore, it is of crucial importance to capture a more realistic picture of thermal conductivity of these nanosheets. Polycrystalline BC_3NS ($PCBC_3NSs$ are herein simulated by Molecular Dynamics simulation to take their thermal conductivity fingerprint applying ΔT of 40K. A series of $PCBC_3NSs$ were evaluated for thermal conductivity varying the number of grains (3, 5, and 10). The effect of grain rotation was also modeled in terms of Kapitza thermal resistance per grain, varying the rotation angle ($\theta/2$=14.5, 16, 19, and 25°). Overall, a non-linear temperature variation was observed for $PCBC_3NS$, particularly by increasing grain number, possibly because of more phonon scattering (shorter phonon relaxation time) arising from more structural defects. By contrast, the heat current passing across the slab decreased. The thermal conductivity of nanosheet dwindled from 149$Wm^{-1}K^{-1}$ for monocrystalline BC_3NS to the values of 129.67, 121.32, 115.04, and 102.78$Wm^{-1}K^{-1}$ for $PCBC_3NSs$ having 2, 3, 5, and 10 grains, respectively. The increase of the grains rotation angle (randomness) from 14.5° to 16°, 19° and 25° led to a rise in Kapitza thermal resistance from $2\times10^{-10}m^2K\cdot W^{-1}$ to the values of 2.3×10^{-10}, 2.9×10^{-10}, and $4.7\times10^{-10}m^2K\cdot W^{-1}$, respectively. Thus, natural 2D structure would facilitate phonon scattering rate at the grain boundaries, which limits heat transfer across polycrystalline nanosheets.