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An atomistic study on thermal transport in B-C-N graphitic systems and heterojunctions: Influence of concentration and temperature.

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Over the last years, two-dimensional graphitic materials composed of B-C-N have attracted remarkable interest because these systems offer a new and broad field to explore and develop nanoscale devices with tunable properties. In this scenario, the thermal conductivity, the temperature profile, the Kapitza resistance and the thermal rectification become the measurable physical quantities that characterize the thermal transport. In the present work, we investigate the influence of C concentration (10-90%) and temperature dependence (100-700 K) in B-C-N graphitic systems. For this, non-equilibrium molecular dynamic simulations were carried out using the LAMMPS code. The results show that thermal conductivity is strongly influenced by C concentration and temperature in B-C-N systems. On the contrary, there is no clear difference in the temperature profile by varying the C concentration. On the other hand, in other graphitic systems, such as graphene heterojunctions, at 100 K, thermal rectification takes its maximum value of 78%, 13% and 50% for interfaces made of hBN, hSiC and Graphane, respectively. Also, Kapitza resistance decreases when the temperature increases up to 700 K. The opposite occurs for thermal conductivity, which shows a value of 100, 50 and 50 W/m-K for the hBN, hSiC and Graphane interfaces at 700 K, respectively.

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