Electrical and thermal transport in coplanar polycrystalline graphene-hBN heterostructures

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We present a theoretical study of electronic and thermal transport in polycrystalline heterostructures combining graphene (G) and hexagonal boron nitride (hBN) grains of varying size and distribution. By increasing the hBN grain density from a few percent to 100%, the system evolves from a good conductor to an insulator, with the mobility dropping by orders of magnitude and the sheet resistance reaching the MΩ regime. The Seebeck coefficient is suppressed above 40% mixing, while the thermal conductivity of polycrystalline hBN is found to be on the order of 30-120 $Wm^{-1} K^{-1}$. These results, agreeing with available experimental data [1], provide guidelines for tuning G-hBN properties in the context of two-dimensional materials engineering. In particular, while we proved that both electrical and thermal properties are largely affected by morphological features (e.g., by the grain size and composition), we find in all cases that nanometer-sized polycrystalline G-hBN heterostructures are not good thermoelectric materials [2].

References

[1] Y. Gong et al. Nat. Commun. 5, (2014) 3193.

[2] J.E. Barrios Vargas et al. Nano Lett., 17, 3, (2017) 1660-1664.

Figures

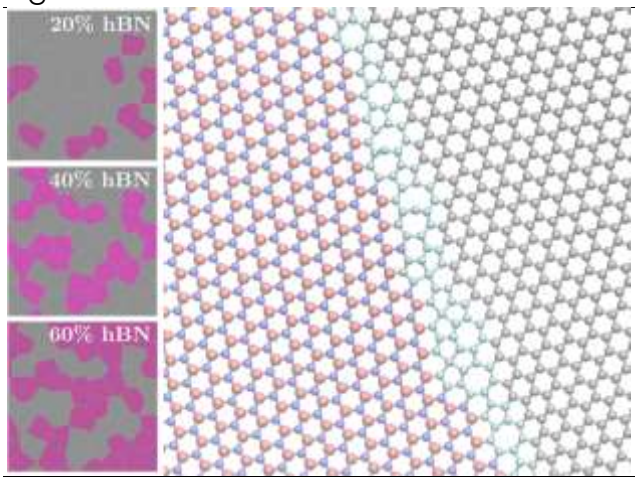

Figure 1: Left panel: square periodic polycrystalline structures with three different concentrations of hBN (20%, 40%, and 60%). Right panel: magnification of the polycrystalline structure showing a typical interface between graphene and hBN grains.

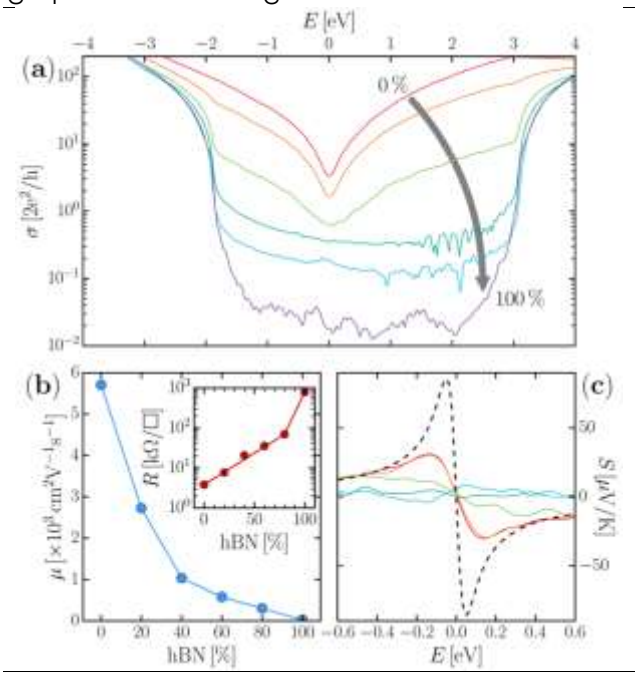

Figure 2: (a) Conductivity vs energy for various hBN grain densities, with an average grain size of 40 nm. (b) Mobility as a function of hBN concentration for a fixed carrier density n = 0.3 × 10^{12} cm^{-2}. Inset: the sheet resistance for the same carrier density. (c) Seebeck coefficient with increasing hBN grain density, with the dashed line showing the pristine graphene value.