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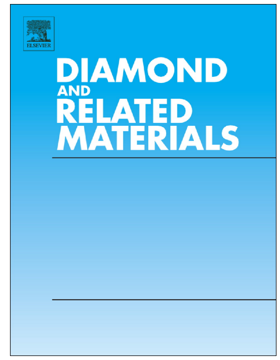

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Thermal Conductivity, Heat Capacity and Magnetic Susceptibility of Graphene and Boron Nitride Nanoribbons

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Using the Kubo-Greenwood formula based on Green's function method and modified third nearest neighbor tight-binding approximation based on density functional theory (DFT) calculations, the electronic properties and temperature dependence of thermal conductivity, heat capacity and magnetic susceptibility of GNRs and BNNRs are calculated in presence of electric field. By increasing the electric field, the band gap of GNRs are approximately constant then decreases to zero, unlike to the band gap of BNNRs which decreases linearly to zero with increasing the electric field. The thermal conductivity, κ(T) for all structures increases with temperature to its maximum value and then decreases by further temperature increasing. In the lower (higher) temperature ranges, the electric field increases (decreases) the κ(T) for all structures. The thermal conductivity of A-BNNR is smaller (larger) than that of A-GNR in the lower (higher) temperature range. Both GNR and BNNR systems have schottky anomaly and their heat capacity increases before schottky anomaly peak and decreases after it. For Both GNR and BNNR systems, the magnetic susceptibility, χ(T) increases with temperature and the χ(T) of A-GNR is larger than χ(T) of A-BNNR.

Keywords: Graphene Nanoribbons, Borom Nitride Nanoribbons, Tight Binding, Thermal Conductivity, Heat Capacity, Magnetic susceptibility