

Transient Thermal Behavior of Graphene under Thermal Impulse

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A transient molecular dynamics technique is developed to characterize the thermophysical properties of two-dimensional graphene nanoribbons (GNRs). By directly tracking the thermal relaxation history of GNR that is heated by a thermal impulse, we are able to determine its thermal diffusivity fast and accurate. We study the dynamic thermal conductivity of different length GNRs of 1.99 nm width. Quantum correction is applied in all the temperature calculations and is found to have a critical role in thermal transport study for graphene. The calculated specific heat of GNR agrees well with that of graphite at 300.6 and 692.3 K, showing little effect of the unique graphene structure on its ability to store thermal energy. Strong size effect on GNR's thermal conductivity is observed and its theoretical values for infinite length limit are evaluated by data fitting and extrapolation. With infinite length, the 1.99 nm wide GNR has a thermal conductivity of $149 \text{ W m}^{-1} \text{ K}^{-1}$ at 692.3 K, and $317 \text{ W m}^{-1} \text{ K}^{-1}$ at 300.6 K. Our study of the temperature distribution and evolution suggests that diffusive transport is dominant in the studied GNRs. Non-Fourier heat conduction is observed at the beginning of thermal relaxation procedure. Thermal waves in GNR's in-plane direction are observed only for phonons in the flexural direction (ZA mode). The observed propagation speed ($c = 4.6 \text{ km s}^{-1}$) of the thermal wave follows the relation of (v_g : ZA phonon group velocity). Our thermal wave study reveals that in graphene the ZA phonons transfer thermal energy much faster than longitudinal (LA) and transverse (TA) modes. Also $\text{ZA} \leftrightarrow \text{ZA}$ energy transfer is much faster than the $\text{ZA} \leftrightarrow \text{LA/TA}$ phonon energy transfer.