Molecular Dynamic Simulation of the Thermal Conductivity of Graphene and Graphene Oxide

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The molecular dynamic simulation of the thermal conductivity of one layer and few layer graphene, and graphene oxide has been performed. As the analysis has indicated the main factors which can influence thermal conductivity of graphene paper materials include (1) interplane energy transfer in layered material, (2) intraplane thermal conductivity of each layer, (3) interlayer interaction. We found that for typical sizes of flakes in reduced graphene oxide (GO) about 10 \( \mu \text{m} \) one can expect that interplane energy transfer will not limit the thermal transport, while intraplane thermal conductivity of ideal graphene planes can exceed 3000 W/m-K. However, large concentration of oxygen defects in reduced graphene oxide (about 10 at\%) should result in strong reduction of intraplane thermal conductivity: calculated critical defect density are about 0.1-1% at\%. Thus based on the current knowledge of the structure of reduced graphene oxide one can not assume large thermal conductivity of GO-based materials. More detail analysis of reduced GO structure should be done to understand significance of these defects on thermal transport. Moreover, we show that thermal conductivity of layered materials can be limited by interplane interactions, which results in additional phonon scattering. To prevent these additional scattering one needs to apply careful engineering of interplane structure and direct calculations of influence of this structure on thermal transport in layered materials such as graphene paper.