Enhancement of thermal properties of graphene-based nanofluids

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Conventional liquids such as: water, ethylene glycol, and mixtures of these two are popular and are widely used as coolants for many electronic devices.[1] But, a major problem of these coolants is the low thermal conductivity (0.2-0.6 $WK^{-1}m^{-1}$), which is too small to meet the coming needs and challenges in the field. One way to overcome this barrier is by using solid particles dispersed in fluids to improve their thermal properties.[2,3] The dispersion of nanomaterials is an effective means to enhance the thermal properties of fluids, however, the mechanism behind has not yet been established. In this work, we have developed highly stable surfactant-free graphene nanofluids with enhanced thermal properties based in DMAc, DMF and NMP; and determined the influence of graphene concentration on the thermal conductivity, specific heat capacity, sound velocity and Raman spectra. Results show maximum enhancements of 48% and 18% for the thermal conductivity and specific heat capacity, respectively. The displacement of several Raman bands as a function of graphene concentration in DMAc and DMF suggests that the solvent molecules are able to interact with graphene surfaces strongly indicating a possible local π-π stacking. These interactions together with the naturally formed hydrogen bonds between DMAc and DMF molecules create a dynamic order, in which graphene acts as an "accelerating centre" for thermal waves. As far as we are aware this is the first time that a mechanism behind *k* enhancement in NFs is proposed and supported by both experimental and theoretical simulations. Our study provides considerable insight into the field of thermal transport in dynamic systems, as liquids and NFs, addressing a fundamental problem in NFs. DFT and MD methods were applied to shed light on the spectroscopic results. The calculations showed that the most frequent DMF orientation with respect to graphene was the parallel one. We found that three parallel configurations presented the highest occurrence. Later, these configurations were used as an input for DFT simulations. It showed that these configurations were the most energetically favourable, facilitating π-π stacking. For the Case of NMP, we did not find any significant modification on the thermal properties and/or in the Raman spectra. Suggesting that the enhancement of thermal conductivity for these fluids is strongly correlated with the displacement of these Raman modes.

References

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