Fundamentals of thermal properties of amorphous sp2 carbon monolayers

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In a recent experiment breakthrough, the synthesis of wafer-scale two-dimensional amorphous carbon monolayers have been reported. This new material seems to present unprecedented properties when integrated as coating of metals, semiconductors or magnetic materials, hence opening a new dimension for atomic layer deposition and ultracompact technologies. Here, we propose a structural characterization of the structural degree of amorphousness of such carbon membranes which could be controlled during the growth phase. We identify how energy is dissipated in such system by a systematic analysis of emerging vibrational modes whose localization increases with the loss of spatial symmetries, resulting in tunable thermal conductivity varying by more than one order of magnitude. Our simulations provide some recipe to design most suitable “amorphous graphene” (am-G) based on the target applications such as ultrathin heat spreaders, energy harvesters or insulating thermal barriers.
Specifically, using MD we design large scale models of disordered sp2 carbon monolayers with a varying degree of amorphousness. We characterize the degree of disorder in real space and k-space and follow how vibrational properties evolve with increasing the loss of crystallinity. We identify the class of phonon modes emerging in such structures, and connect their emergence with the resulting thermal properties of those membranes. Compared to the pristine graphene value, by tuning the crystalline order, the thermal conductivity is found to vary by more than one order of magnitude, although remaining quite high compared to other forms of amorphous materials.

References

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Figures

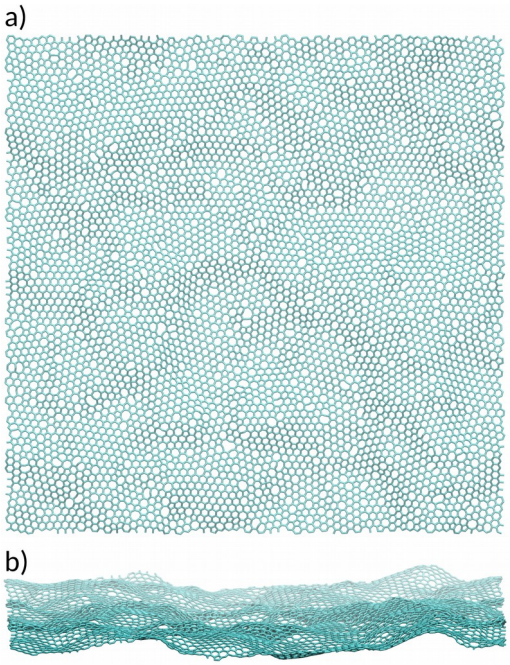

Figure 1: Am-G sample.

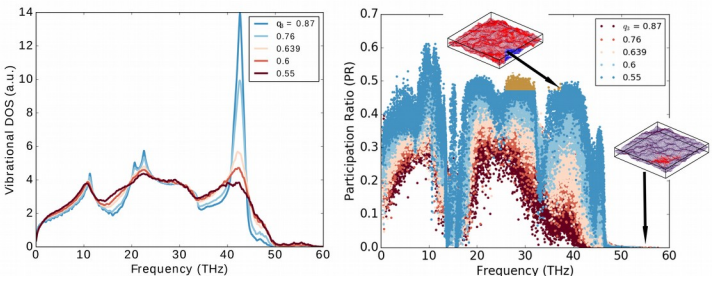

Figure 2: (Left) Vibrational DOS of Am-G for different degrees of amorphousness. (Right) Participation Ratio of the samples and atomic displacements (insets).