On the Vibrational and Thermal Properties of Amorphous Graphene: an atomistic investigation

Aleandro Antidormi[1] , Stephan Roche[1,2]
[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193, Barcelona, Spain*
[2] *ICREA Institucio Catalana de Recerca i Estudis Avancats,* 08010 Barcelona, Spain
aleandro.antidormi@icn2.cat

Amorphous materials are used in a wide range of applications, but their atomic-scale structure and its effect on properties are far more complex than those of crystalline analogues. Among the large family of 2D amorphous materials, amorphous Graphene (am-G) has emerged as an extremely promising candidate due to recent advancements in the fabrication process. Amorphous carbon monolayers on Ge substrates using conventional chemical vapour deposition (CVD) have been sinthesized at high temperatures resulting in a material with strong Anderson insulating behaviour and a unique ability as an atom-thick interface layer [1]. More recently, the synthesis via laser-assisted chemical vapour deposition of centimeter-scale, free-standing, continuous monolayer of amorphous graphene was also reported, with potential application for permeation and diffusion barriers in flexible electronics [2].
It is clear that the properties of amorphous graphene are a consequence of both the nature and the amount of disorder (degree of amorphousness) in the atomic configuration of the material. Being the amount of disorder mostly related to the synthesis parameters in the fabrication process, it represents a tunable parameter which can be ideally used to control its physical properties. This poses the need for a systematic investigation of the properties of a-G as a function of the degree of amorphousness.
In this study we focus on the vibrational and thermal properties of Am-G providing a systematic analysis of the vibrational modes in a-G samples as a function of the degree of amorphousness. Following the pioneering work by Allen and Feldman [3] on amorphous silicon, we propose for such modes a classification into extended modes (diffusons and propagons) and localized vibrations (locons). The effect of amorphousness on the density of states, the participation ratio, and the intrinsic character of the vibrational modes is given. Finally, the contribution of each single mode to the overall thermal conductivity is calculated, highlighting the most effective vibrations responsible for heat transport in am-G.

References

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[3] Allen, P. B., et al. , *Philosophical Magazine B* 79.11-12 (1999): 1715-1731.

Figures

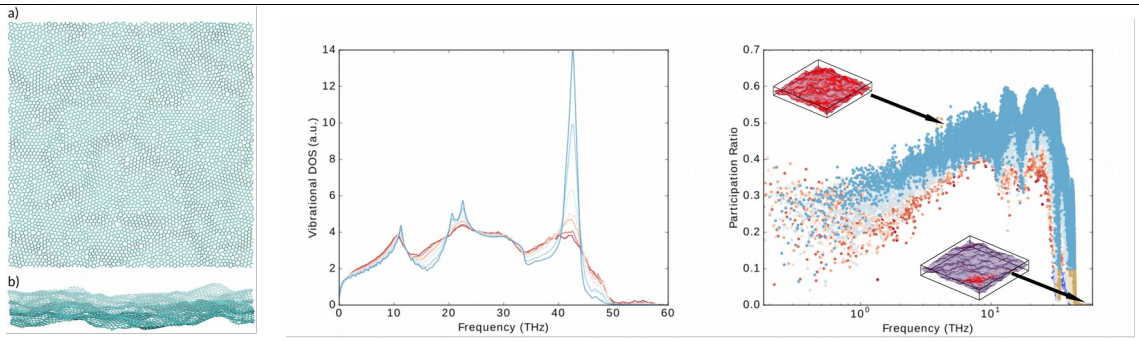

Figure: (Left panel) Am-G sample. (Center panel) Vibrational density of States of Am-G samples for different degrees of amorphousness. (Right panel) Participation Ratio of the samples as a function of frequency. (Inset) Atomistic displacements of a diffuson and a a locon modes.