What are amorphous 2D Materials good for?

Stephan Roche
[1]Catalan Institute of Nanoscience and Nanotechnology (ICN2), Bellaterra, 08193, Barcelona, Spain
[2] ICREA Institucio Catalana de Recerca i Estudis Avancats, 08010 Barcelona, Spain

stephan.roche@icn2.cat

Abstract

Amorphous materials such as boron nitride (aBN) and amorphous graphene (aG) are becoming prominent materials for many different applications due to their good properties such as thermal stability, mechanical properties, insulating behavior, and ultralow dielectric constant in aBN (<2). Moreover, amorphous films are more suitable to large area deposition compared to clean hBN or graphene since it can be grown at low temperatures (about 400 ºC) and on various substrates [1-3]. However, their properties depend on the nature and degree of disorder, which needs a well-defined metrics for benchmarking materials. Having such metrics in place will allow to tune the properties and performance of these films during the fabrication for desired applications. In this context, revealing the relationship between fabrication strategies and the material properties of the film is also crucial.

Capturing the key features of the amorphous nature of materials requires theoretical characterization to understand how material properties change with the microstructure. Since simulations of amorphous materials need large structural models, density functional theory (DFT) is not a suitable tool despite the high accuracy it offers. On the other hand, molecular dynamics (MD) simulations with empirical interatomic potentials require much less computational cost; however, they are not accurate enough to correctly describe the local environment of amorphous materials. Machine learning-driven interatomic potentials (ML-IP) can describe the local environment with a similar accuracy to DFT and at a much lower cost [4,5]. Here, we introduce Gaussian approximation potentials (GAP) for atomistic simulations of aBN incorporating different contaminators and doping materials, which are trained on a large dataset of atomic structures generated by DFT calculations [6-8]. We will present a systematic analysis to screen out possible realistic morphologies as a function of growth parameters, such as temperature, quenching rate, and the presence of a dopant, and their corresponding material properties using GAP-driven MD simulations. The extensive simulations of a large quantity of possible structures presented in this work will guide experimental research and provide trends of scaling behavior as a function of experimentally controllable parameters. The impact of amorphousness on dielectric properties will be also discussed for aBN and aG [9,10].

References

[1] Hong, S et al. Nature 582, 511–514 (2020). DOI: 10.1038/s41586-020-2375-9.
[2] Glavin, N. R., et al., Adv. Func. Mat. (2016). DOI: 10.1002/adfm.201505455.
[3] Chen, C. Y., et al., arxiv: 2312.09136 (cond-mat).
[4] Unruh, D., Meidanshahi, RZ., Goodnick, SM., Csányi, G. and Zimányi GT. Physical Review Materials 6, 065603 (2022). DOI: 10.1103/PhysRevMaterials.6.065603.
[5] Deringer, VL. and Csányi, G. Physical Review B 95, 094203 (2017). DOI: 10.1103/PhysRevB.95.094203.
[6] Kaya, O., et al. Nanoscale Horizons 8, 361–367 (2023). DOI: 10.1039/D2NH00520D.
[7] Kaya, O. et al. arXiv:2310.18102 (cond-mat).
[8] Kaya, O. et al. arXiv:2402.01251 (cond-mat).
[9] Th. Galvani et al. arXiv:2403.11924 (cond-mat).
[10] Th. Galvani, O. Kaya, S. Roche, unpublished

Acknowledgments

We acknowledge FLAGERA MINERVA and Proyecto PCI2021-122092-2A financiado por MICIU/AEI /10.13039/501100011033 y por la Unión Europea NextGenerationEU/PRTR

Figure

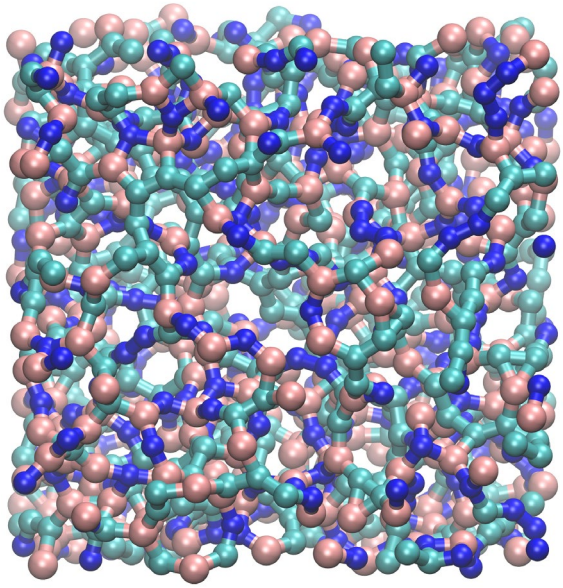

Figure 1. Typical amorphous structure of aBN:C compounds, namely an amorphous BN structure with a certain density of carbon atoms, affecting the overall system properties (thermal stability, mechanical and dielectric properties, etc)