Machine Learning Driven Molecular Dynamics Simulations to Explore the Properties of Amorphous Boron Nitride

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Abstract

Amorphous boron nitride (aBN) is a prominent material for many different applications due to its excellent properties such as great stability, good mechanical properties, being a good insulator, having ultralow dielectric constant (<2). Moreover, aBN films are more suitable to large area deposition compared to hBN since it can be grown at low temperatures (65-400 °C) and on various substrates [1-3]. However, its properties depend on the nature and degree of disorder. This allows us 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 crucial.

The amorphous nature of the material 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]. In this talk, I 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.

References

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