Revealing Structure-Property Relationships in Amorphous Boron Nitride Using Machine-Learned Potentials

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Abstract

Amorphous boron nitride (aBN) is a key material for next-generation electronic devices, particularly as an ultralow dielectric material and diffusion barrier in semiconductor technology due to its high thermal stability, mechanical strength, and low dielectric constant[1,2]. However, a comprehensive understanding of its atomic structure is essential to optimise performance yet remains challenging both experimentally and theoretically. In particular, the amorphous nature of the material makes theoretical characterisation necessary to understand how material properties change with the microstructure, and to connect processing conditions to realistic atomic-scale morphologies.

Because they lack long-range order, traditional experimental methods such as XRD and NMR provide only limited statistical insights into the local atomic environments of amorphous materials. These techniques cannot directly resolve atomic structures, leaving many details ambiguous. This limitation hinders our understanding of the structural properties of amorphous materials. On the theoretical side, simulating amorphous materials requires balancing accuracy with computational feasibility. Classical force fields, although efficient, often fail to capture the complexities of disordered systems, whereas density functional theory (DFT), though accurate, is computationally expensive and limited to small system sizes [3-5]. Since simulations of amorphous materials require large structural models to obtain representative local environments, DFT alone is not a practical tool for systematic screening of processing conditions.

To address these challenges, we developed a machine learning model using Gaussian Approximation Potential (GAP), trained on a DFT-generated dataset [5]. More broadly, machine learning-driven interatomic potentials can describe local atomic environments with an accuracy comparable to DFT but at a much lower computational cost, enabling extensive molecular dynamics (MD) simulations beyond the reach of direct DFT. This GAP model enables large-scale amorphous structure simulations with near-DFT accuracy, bridging precision and efficiency. Using melt-quench simulations, we generated realistic atomistic models of aBN, which closely match experimental diffraction patterns and structural factors. Later, we perform a systematic analysis to screen realistic morphologies as a function of growth parameters and evaluate the corresponding materials properties using GAP-driven MD simulations. This method captures the short- and medium-range order in aBN, providing a detailed structural model that surpasses experimental techniques alone. Additionally, this approach offers a framework applicable to other amorphous and disordered materials, unveiling the principles governing their formation. Our findings provide valuable insights into the atomic structure of aBN, paving the way for future research and applications in electronics and nanotechnology.

References

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