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

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Abstract

Amorphous boron nitride (aBN) has garnered significant attention for its potential applications in advanced electronics, particularly as an ultralow dielectric material and a robust diffusion barrier in semiconductor technology. Combining high thermal stability, mechanical strength, and desirable electronic properties, aBN is a leading candidate for next-generation devices, where minimising electronic interference and enhancing durability are critical [1]. However, a complete understanding of its atomic structure is essential to optimise its performance. This remains a significant challenge due to the lack of long-range order in amorphous materials, which complicates both experimental characterisation and theoretical modelling.

Traditional experimental methods, including X-ray diffraction (XRD) and nuclear magnetic resonance (NMR), provide only statistical insights into local atomic environments, leaving many structural details unresolved [2]. Computational methods face their own limitations, while classical force fields fail to capture the complexities of disordered systems, density functional theory (DFT), though accurate, is computationally prohibitive for large-scale simulations [3]. These limitations restrict our ability to fully map the atomic configurations in aBN, hindering progress in understanding its structure-property relationships.

To address these challenges, we employed a Gaussian Approximation Potential (GAP) [4], a machine-learned interatomic model trained on high-quality DFT datasets [5,6]. GAP enables simulations that achieve near-DFT accuracy while scaling to system sizes inaccessible to DFT. Using melt-quench molecular dynamics, we generated realistic structural models of aBN that align closely with experimental data, such as diffraction patterns and structural factors. These simulations reveal both short- and medium-range atomic ordering, offering a detailed understanding of the disordered network. Furthermore, this approach provides a clearer link between atomic-scale morphology and material behaviour, addressing long-standing gaps in the characterisation of amorphous materials.

This study demonstrates the capability of machine-learned potentials to overcome key limitations in modelling disordered systems, bridging the divide between computational feasibility and accuracy. The methods and insights developed here not only deepen our understanding of aBN but also establish a transferable framework for investigating other amorphous materials. These findings pave the way for future research and practical applications in electronics and nanotechnology, where advances in materials design remain a priority.

References

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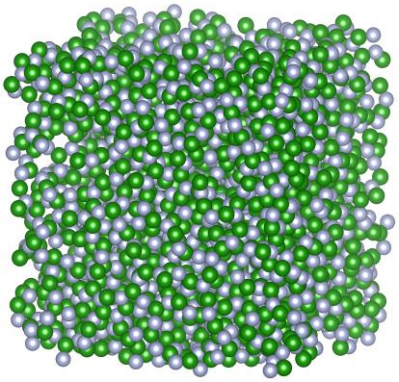

Figure: Melt-quench aBN sample.