# Unveiling the Atomic Structure of Amorphous Boron Nitride Films

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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.

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, whilst 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].

To address these challenges, we developed a machine learning model using Gaussian Approximation Potential (GAP), trained on a DFT-generated dataset [5]. 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. 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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