Amorphous Boron Nitride: Atomistic Characterization and Performances

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Abstract

Amorphous boron nitride (aBN) has been revealed as an ultralow dielectric constant material (κ<2), with strong thermal stability and mechanical properties, making it highly suited for next generation interconnects technologies [1, 2]. The uniqueness of amorphous materials derives from their complex structure, which can to some degree be controlled at the fabrication level, and allows the tuning of specific properties useful for applications. In this respect, new fabrication strategies to modify the structural properties and a systematic theoretical characterization of the impact of the thermal, mechanical and electronic properties are urgent. In this work, we present a theoretical investigation of thermal and mechanical properties of aBN as a function of external parameters such as temperature, quenching rate, presence of unwanted or dopant atoms. Using machine learning interatomic potentials, we ensure the reliability of our calculations by describing the atomic interactions more accurately, introducing Gaussian Approximation Potentials [3] which are trained on a large dataset of atomic structures generated with ab-initio calculations [4,5]. We found that the incorporation of dopant atoms causes a significant change in the structure of aBN, which is strongly reflected in the resulting the thermal and mechanical properties of the compounds [4]. Further, we will discuss the anticorrosive properties and dielectric constant of aBN films. Our simulations will provide some recipe to design most suitable amorphous boron nitride-based coatings and metal diffusion barriers.

References

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Figures

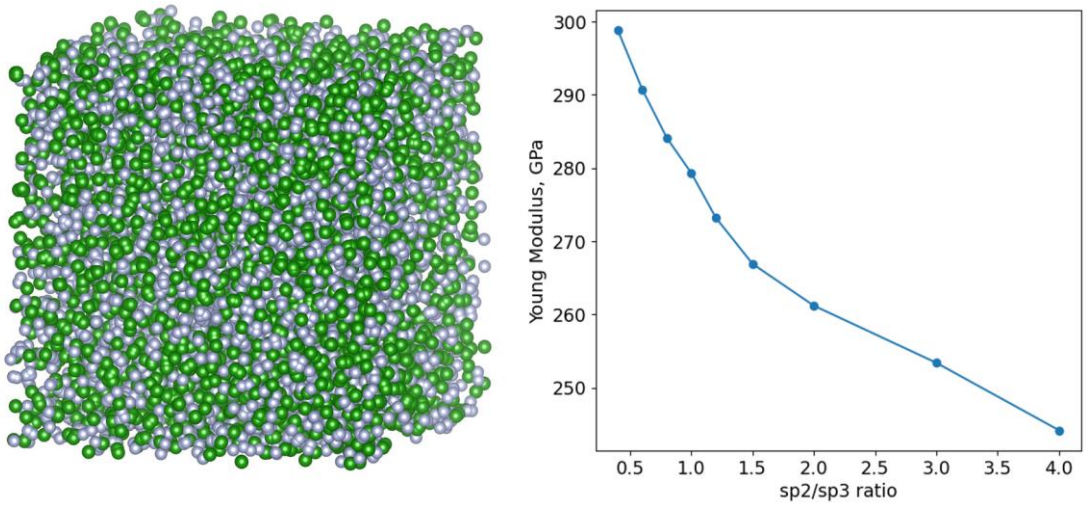

Figure 1: A ball-and-stick picture of aBN sample (left) and Young's Modulus of aBN samples with varying sp^2/sp^3 bond ratio (right).

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