Revealing the Thermal and Mechanical Properties of Amorphous Boron Nitride

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ABSTRACT

Interconnect materials with ultralow dielectric constant, good thermal and mechanical properties are crucial for further miniaturization of electronic devices. Recently, it is demonstrated that ultrathin amorphous boron nitride (aBN) films have very low dielectric constant ($\kappa<2$), high density (above 2.1 g/cm^3), high thermal stability and mechanical properties. Additionally, it is more suitable for large area deposition compared to its crystalline counterparts, since it can be grown lower temperature, which opens new integration opportunities with 2D materials into flexible devices for nanoelectronics and spintronics [1,2].

The excellent properties of aBN derives from the nature and degree of disorder, which can be controlled at fabrication, allows to tune the physical properties for desired applications. In this context, new fabrication strategies to modify the structural properties and a systematic theoretical characterization of the impact of structural properties on the performance of the material is crucial.

In this work, we will present a systematic analysis to screen out possible realistic morphologies as a function of growth parameters, such as temperature, quenching rate and presence of dopant, and their corresponding thermal and mechanical properties using classical molecular dynamics simulations. We ensure the reliability of results by introducing Gaussian Approximation Potentials which are trained on a large dataset of atomic structures generated by ab-initio calculations. We found that quenching rate and level of dopants causes a significant change in structural properties of aBN, which is strongly reflected in the resulting mechanical and thermal properties of the compounds. We believe the extensive simulations of 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. We will also mention the anticorrosive properties of the material against oxidation.

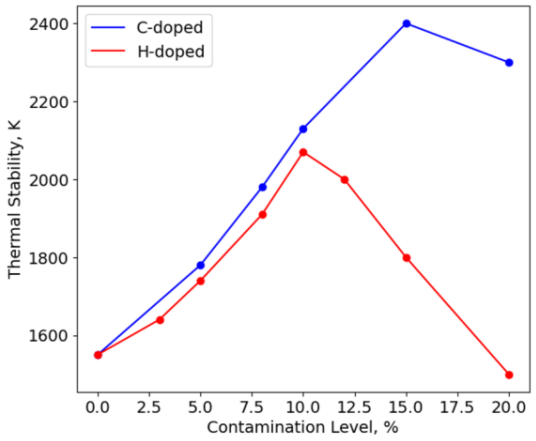

Fig. 1. Thermal stability of amorphous boron nitride as a function of level of contamination.

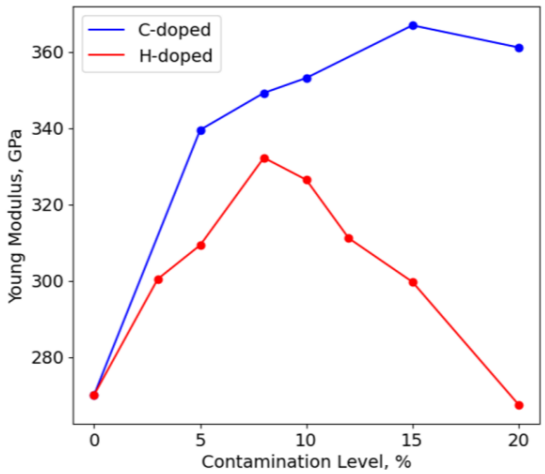

Fig. 2. Young's Modulus of amorphous boron nitride as a function of level of contamination.

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