Impact of Carbon and Hydrogen Doping on Stability and Mechanical Properties of Amorphous Boron Nitride

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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 this material suited for next generation interconnects technologies [1, 2]. The uniqueness of amorphous materials derives from the inherent imperfect structure nature, which can be controlled at fabrication level, represents the key ingredient for specific target applications. In this respect, new fabrication strategies to modify the structural properties and a systematic theoretical characterization of the impact of the structural properties on thermal stability and mechanical properties are urgent. In this talk, a theoretical investigation of thermal and mechanical properties of aBN as a function of varying external parameters such as temperature, quenching rate, presence of unwanted or dopant atoms using molecular dynamic simulations will be presented. Using machine learning technique, we ensure the reliability of calculations of properties by first describing the atomic interactions more accurately, introducing two Gaussian Approximation Potentials [3] (for aBN:C and aBN:H) which are trained on a large dataset of atomic structures which generated ab-initio calculations [4,5]. We found that then incorporation of both C and H atoms causes a significant change in atomic environment of aBN, which is strongly reflected in the resulting the thermal stability and mechanical properties of the compounds [4]. We will also discuss the antioxidation properties of aBN.

References

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Figures

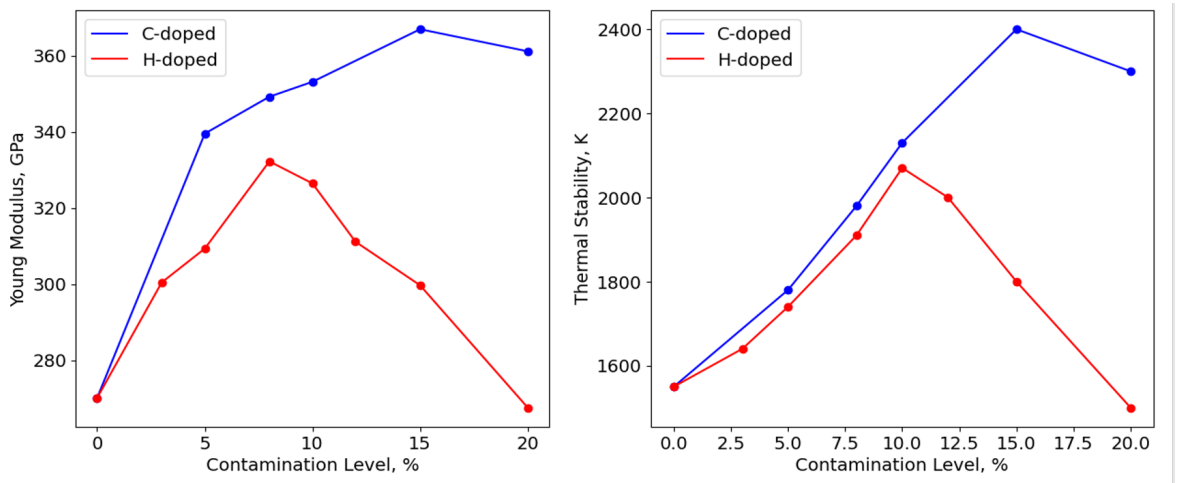

Figure 1: Young's modulus and thermal stability of C- and H-doped amorphous boron nitride.

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