Investigation of Microstructure and Stability of Amorphous Boron Nitride upon Carbon Contamination

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Abstract

The development of barrier materials with low dielectric constant, good thermal and mechanical properties is the key to progress in further miniaturisation of interconnects and downscaling microelectronics. A recent study [1] shows that amorphous boron nitride (aBN) possesses very low dielectric constant and low metal diffusivity and high mechanical robustness. Moreover, since it can be grown at much lower temperatures than its hexagonal counterpart (hBN), its integration in silicon-based devices is much easier. Even though the excellent properties of atomically thin aBN shows that it has great potential for barrier applications, we need a deeper understanding of its microscopic structure and its relationship with device performance. In this study, the effect of varying level of carbon (C) contamination on structural, thermal, and mechanical properties of aBN are investigated using classical molecular dynamics, given that C is one of the typical contaminants in dielectrics grown at lower temperature. To ensure the reliability of calculations and describe the atomic interactions more accurately, a Gaussian Approximated Potentials (GAP) is trained on a large dataset of atomic structures which obtained via ab-initio calculations [2]. We report that C contamination of aBN samples causes a significant change in thermal stability and mechanical properties.

References

[1] Hong, S., Lee, CS., Lee, MH. et al. Nature 582 (2020) 511–514.
[2] Bartók, A. P., Payne, M.C., Kondor, R, Csányi, G. Physical Review Letters, 104 (2010) 136403. Bartók, A. P., Csányi, G. Quantum Chem. 115 (2014), 1051– 1057.
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Figures

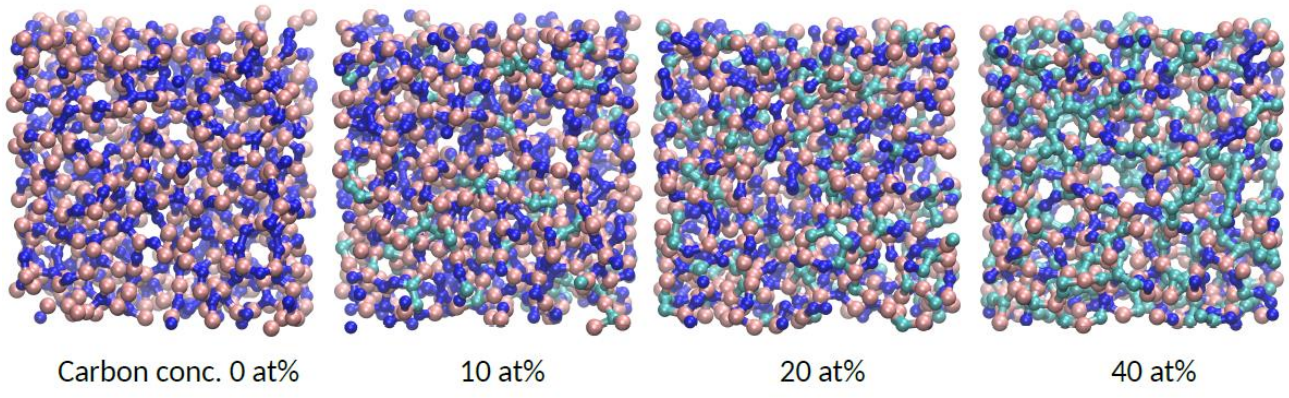

Figure 1: aBN samples with different level of C concentration.