Dielectric properties in models of amorphous Boron Nitride

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The increasing demand for data storage and processing calls for improvements in computing hardware. One of the challenges in this path is that RC delays from interconnects in integrated circuits do not scale with device dimension, therefore requiring new materials with reduced dielectric constants [1]. Recent reports of amorphous Boron Nitride (aBN) as an ultralow dielectric constant material with good mechanical and thermal properties and a low growth temperature have thus sparked considerable interest [2], as have its promising applications as a dielectric material for two-dimensional systems [3].

In this work [4], we theoretically investigate the electronic and dielectric properties of aBN based on machine learning structural models [5], and attempt to correlate them to the samples' atomic structures.

Indeed, as an amorphous material, the properties of aBN depend strongly on its atomic structure, which can be acted upon through fabrication parameters. Because of the complexity of these atomic structures, the precision required for their description and the need to consider large unit cells, we leverage molecular dynamics with machine learned interatomic potentials (MLIPs) [5] to obtain them.

We first generate a dataset of small structures (~100 atoms), whose electronic properties are accessible to DFT, from which correlations between structural characteristics and dielectric constants were extracted. As DFT, while precise, is limited in sample size, we supplement this by the study of larger and more realistic structures (~10.000 atoms) with a simple tight-binding model, providing qualitative access to large-scale disorder and localization effects.

Our results point at the existence of disorder-induced "mid-gap" states, which may increase aBN's dielectric constant. For small samples, the lowest dielectric constants were typically obtained for stoichiometric (B/N=1), sp2-dominated samples with strong short-range order [6]. Concurrently, we found that large structures exhibited localization effects and a reduction in their transitions' oscillator strengths which relates to their amorphous nature and lowers their dielectric constant compared to a reference crystalline structure.

On these grounds, we further reflect on the need for machine learning techniques to predict tight-binding Hamiltonians [7]. Such methods, allied to MLIPs for structure prediction and linear scaling methodologies for the computation of properties of merit [7,8] could improve electronic structure prediction by bridging the gap from high precision *ab initio* methods towards a more holistic characterization of large and complex disordered systems of technological interest, like aBN.

References

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Figures

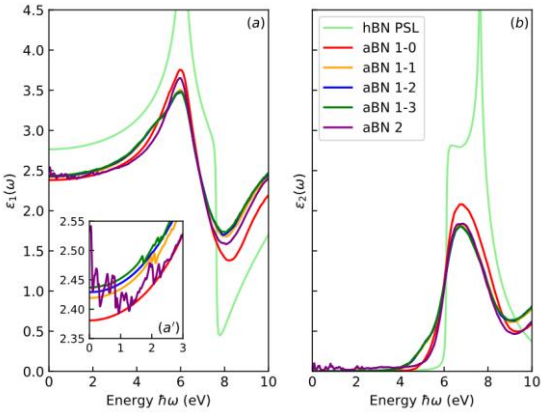

Figure 1. Dielectric functions of MLIP-generated aBN structures computed using tight-binding ((a): real part; (b): imaginary part) [4].