Exploring Dielectric Properties in Models of Amorphous Boron Nitride

Thomas Galvani[1]
Ali K. Hamzee[2], Laura Caputo[3], Onurcan Kaya[1,4], Simon Dubois[3], Luigi Colombo[6], Viet-Hung Nguyen[3], Yongwoo Shin[2], Hyeon-Jin Shin[5], Jean-Christophe Charlier[3] and Stephan Roche[1,7].
[1] *Catalan Institute of Nanoscience and Nanotechnology (ICN2), CSIC and BIST, Campus UAB, Bellaterra, 08193, Barcelona, Spain*
[2] *Advanced Materials Lab, Samsung Semiconductor Inc., Cambridge, MA 02138, USA*
[3] *Institute of Condensed Matter and Nanosciences, Université catholique de Louvain (UCLouvain), Chemin des Étoiles 8, Louvain-la-Neuve 1348, Belgium*
[4] *School of Engineering, RMIT University, Melbourne, Victoria, 3001, Australia*
[5] *Department of Semiconductor Engineering, School of Electrical Engineering and Computer Science, Gwangju Institute of Science and Technology (GIST), Gwangju 61005, Republic of Korea*
[6] *CNMC, LLC, Dallas, TX, 75248, USA*
[7] *ICREA Institucio Catalana de Recerca i Estudis Avancats, 08010 Barcelona, Spain*
thomas.galvani@icn2.cat

As the need for data storage and processing booms, improvements in computing hardware are crucially needed. One challenge is that the RC delay of interconnects, compared to the RC delay of transistors, does not scale with device dimension, resulting in a bottleneck for integrated circuits performance [1]. There is thus a need for the development of new materials to optimize interconnects through dielectric constant and metal resistivity reduction. In this context, recent reports of amorphous Boron Nitride (aBN) as an ultralow dielectric constant material with remarkable mechanical and thermal stability have sparked great interest [2]. In this work [3], we present a theoretical study of aBN's electronic and dielectric properties, and correlate them to its atomic structure. Indeed, as an amorphous system, the performance of aBN hinges on its structure, which can be acted upon through fabrication parameters. We first generate a set of small (~100 atoms) aBN structures using machine learned force-fields [4] and explore their properties using *ab initio* techniques (DFT). In this way, we extract correlations between the samples' dielectric constants and their bonding (sp1/2/3) and disorder (B-N alternation) characteristics as well as their chemical makeup (B/N ratio). Because this approach, while precise, is limited in sample sizes, we concurrently employ a simple tight-binding model to investigate larger and more realistic structures (~10.000 atoms), allowing us to qualitatively study the effects of localization and large-scale disorder. Our results point at the existence of disorder-induced "mid-gap" states, which increase aBN's dielectric constant. For small samples, the lowest values were typically obtained for sp2-dominated structures with B/N=1 and strong short-range order [5]. Simultaneously, we observe in large samples that their amorphous nature induces an overall reduction of their electronic transitions' oscillator strengths compared to a reference BN crystal, which decreases the dielectric constant.

References

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