Atomistic Modelling of Point Defects in Amorphous and Crystalline Phases of Ultra-thin Boron Nitride

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Abstract

Resistive switching architectures are being actively studied for their potential to build the next generation of electronic devices. These architectures are based on a pristine insulator that is sandwiched between two metallic electrodes such that when a voltage difference is applied between both electrodes, a conductive filament is locally formed with a disordered structure. A very strong candidate for this insulator is hexagonal boron nitride (h-BN) due to its large electronic band gap of around 6 eV, among other properties. [1-7] However, the mechanisms for the formation of the conductive filament in h-BN are not yet fully understood. Thus, the goal of this talk is to present our results on the modelling of this conductive filament by evaluating the formation of point defects in hexagonal and amorphous phases. [8] We combine classical molecular dynamics (MD) and density functional theory (DFT) to calculate the formation energy of vacancies in both BN phases. Our calculations with MD indicate that the formation energy for boron vacancies in the crystalline regions is always above 10 eV, a value that reduces to 7.29 and 3.55 eV for the nearest second and third neighbours. On the other hand, the vacancy energy in the amorphous regions shows a much wider stochastic distribution around 4.91 eV and it can reach values down to 0.1 eV. These energies are in very good agreement with the corresponding values of 10.91 and 4.61 eV obtained from DFT calculations on bulk crystalline and amorphous structures. Therefore, the formation of boron vacancies is energetically more favourable in the disordered phase than in its crystalline counterpart. We conclude then that the few-atoms-wide disordered regions in the grown h-BN by chemical vapour deposition represent atomistic loci where electric stress might lead to dielectric breakdown with the resulting creation of conductive channels, in agreement with conductive atomic force microscopy measurements.

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FIGURES

(a) (b)

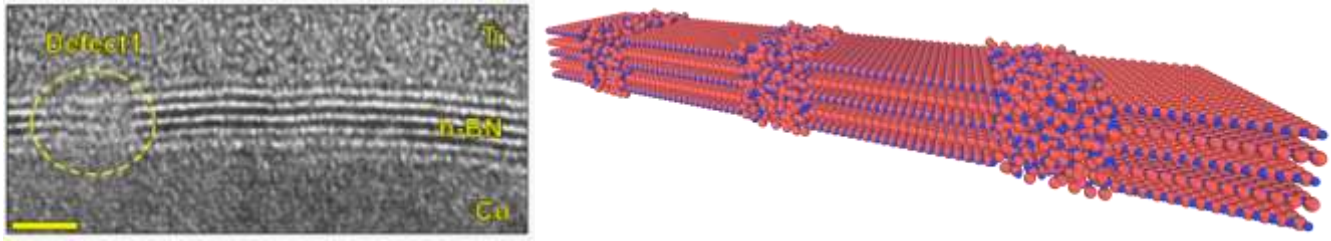

Figure 1: Cross-sectional TEM images of ultra-thin films of hexagonal boron nitride (a) and 3D model of the atomic structure of a multilayer boron nitride.