Grain Boundary Stitching in Hexagonal Boron Nitride – A Theoretical Perspective

Anjali Lalithambika[1]
Ankit Rao[1], Srinivasan Raghavan[1], Manish Jain[2]
1. Centre for Nanoscience and Engineering, Indian Institute of Science, Bangalore, India
2. Centre for Condensed Matter Theory, Department of Physics, Indian Institute of Science, Bangalore, India
Lalithambika.anjali@gmail.com

Abstract: In large-area growth of hexagonal boron nitride (h-BN) for electronic and filtration applications [1], perfect grain-boundary (GB) stitching becomes necessary to ensure mechanical quality and morphological homogeneity across the entire film. Here we inspect theoretically if incompletely stitched GBs can be healed with the introduction of a nitrogen potential. Vacancy defects in a GB are one way by which an incomplete GB stitching can present itself. Here, using density functional theory (DFT) we model nitrogen vacancy defects (Figure 1a) and nitrogen anti-site defects (with boron vacancies at the same points as reference) on an h-BN GB. We choose a GB with 4|8 ring structure as this is reportedly the lowest energy GB structure [2]. PBE [3] ultrasoft pseudopotentials [4], energy cutoff of 60 Ry, and gamma point calculations were used. An 860 atom cell with 15Å vacuum is used to model the GB. Once structures are relaxed Gibb's free energies of formation of the novel point defects were calculated under various nitrogen potentials taking ammonia as the source. The equation for formation energy reads as follows:

$$\Delta G_f = \Delta E_{GB\text{-}vacancy} + n_N \mu_N(NH_3, P_{NH3}, T) - n_H \mu_H(H_2, P_{H2}, T)$$

(Where, $\Delta E_{GB\text{-}vacancy}$ =energy of GB with vacancy minus energy of GB, n_X = the number of atoms of species X, $\mu_X(Y, P_Y, T)$ = chemical potential of species X with Y as source, P_Y = partial pressure of Y, T = the temperature). We firstly find that for typical CVD conditions, $\Delta G_f < 0$ when $P_{NH3} \sim 0$ (Figure 1b), i.e it is thermodynamically possible for these novel point defects to form. We also find that the $\Delta G_f > 0$ for the nitrogen vacancies starting from $P_{NH3} \sim 10^{-20}$ Torr at 1300 K (Figure 1b) meaning they are easily healable.

References

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Figures

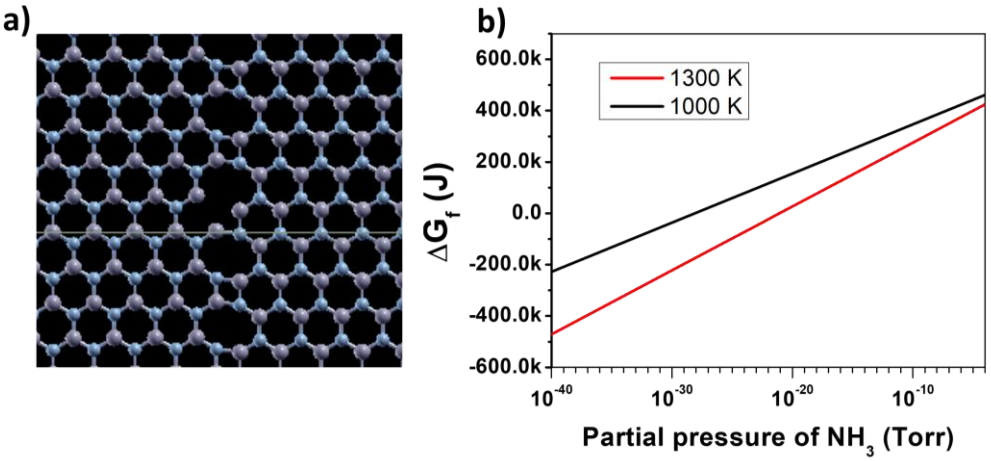

Figure 1: a) Nitrogen vacancy in h-BN GB with 4|8 ring structure (gray & blue balls are boron & nitrogen respectively). b) ΔG_f of the nitrogen vacancy for 1000 K and 1300 K showing negative free energy change at practically zero ammonia partial pressures.