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High Resolution EELS of Point Defects in a Nitride Semiconductor Material

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There is currently considerable interest in B doping of AlN and GaN semiconductors to engineer the band gap for UV laser applications.

We have studied a BAlN thin film grown by MOCVD with gas-flow B/(B+Al) ratio of 18%. The boron content was measured to be ~16% by Rutherford backscattering, but only 9% by X-ray diffraction. The discrepancy has been explained as B segregation at twin boundaries [1]. However, it's also possible that some of boron atoms are on interstitial sites, instead of replacing Al in the film.

Fig 1 shows a high resolution HAADF image of the BAlN film grown on the AlN substrate. It was recorded at 100 kV in the NION HERMES™ 100 with a beam convergence of 30 mrad using the aberration corrector. The position of the atomic columns is well defined in the AlN, but less clear in the BAlN, probably due to defects. The darker regions have higher B concentration, which correlated with maps of intensity in the B K edge.

Transitions involving energy levels associated with point defects are often associated with optical or IR emission, less than 2 eV. These can be resolved with the use of the monochromator in the NION HERMES™ 100, this time operated at 60 kV. A lower accelerating voltage is needed to avoid Cerenkov losses, which would give a background in the bandgap region. Fig 2a shows features with energies ranging from 0.2 to 0.8 eV, recorded by scanning the 11nm x 11nm region shown in Fig 2b. They show a threshold followed by a gradual decrease, similar to that seen for core edges. This is to be expected, as it is possible to excite to higher energy states in the conduction band.

To identify which defects might be responsible for these features, VASP DFT calculations were performed using PAW LDA potentials for single Al, B and N interstitial atoms, and single Al and N vacancies, in a supercell constructed from 3x3x3 AlN unit cells. The structures were initially relaxed with 3x3x3 k points. Subsequently a high-resolution density of states (DOS) was calculated with 5x5x5 k points. The bandgap for AlN from the DOS shown in Fig 3a is underestimated as 4.6 eV, as is typical for DFT. The calculations also determined the position of the Fermi level shown as 0.0 eV, so plausible transitions to the empty states in the conduction band could be identified. Only the B and Al interstitials as shown in Figs 3b and Fig 3c, and N vacancies, showed levels that matched those shown in Fig 2a. Differences between measured energy levels and the DFT results can be attributed to limitations in DFT.

Detection of point defects is the first step in mapping their location at nm resolution, once the functional form of the point spread function is known [2].

References:

[1] S. Wang *et al,* J. Cryst. Growth **475** (2017), p. 334.
[2] The use of facilities within the Eyring Materials Center at Arizona State University is acknowledged.

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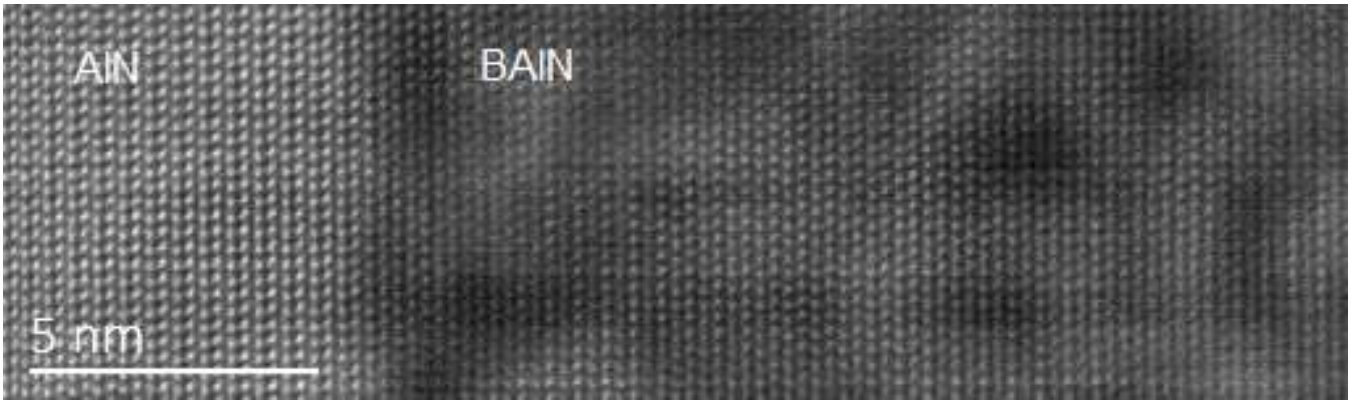

Figure 1. HAADF image showing AlN and B implanted region.

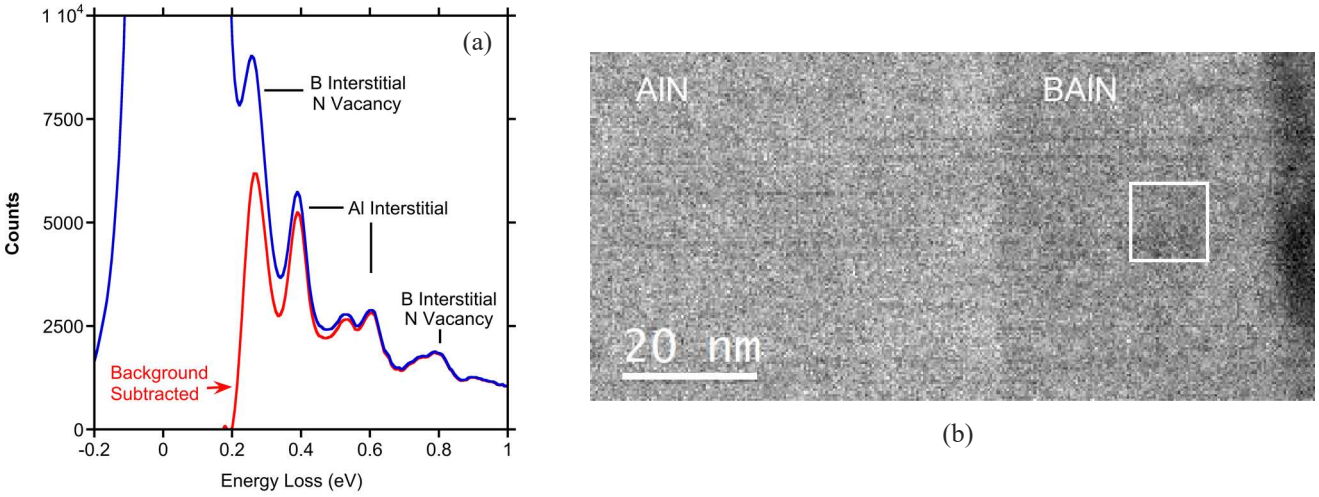

Figure 2. (a) Spectrum features arising from point defects (b) Region from which spectrum was taken.

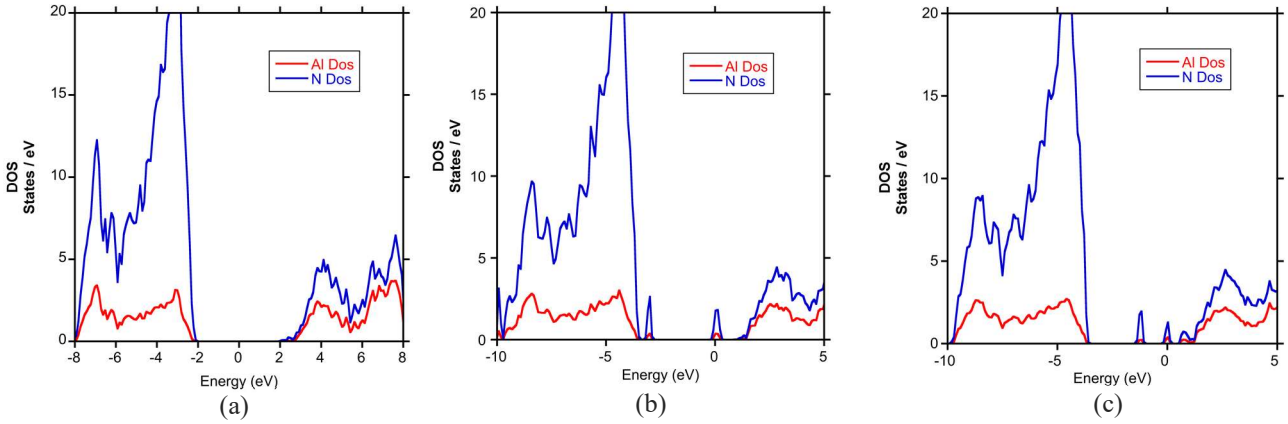

Figure 3. DFT calculations for (a) AlN, (b) with B and (c) with Al interstitial in 3x3x3 supercell.

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