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Access semiconductor bandgaps at atomic resolution?

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Despite that the near-field approaches have claimed a sub-50nm spatial resolution in detection of the materials' optical characteristics; advanced transmission electron microscopy (TEM) in association with delicate valence electron energy-loss spectroscopy (VEELS) remains the selection for its inherent high spatial detectability approaching λ/40, under conservative estimation, where λ represents the excitation wavelength. While applauding for the exciting achievements, questions arise: Can we do it better to implement atomic-level bandgap detection?

It is probably not as straightforward as imagined to pick out a swift conclusion with simply yes or no before understanding the underlying physical picture of VEELS. For energy-losses below 50 eV, VEELS and associated imaging techniques contain material-specific information about volume, surface (or interface) plasmons and single-electron excitations reflecting the dielectric responses of the materials to the electromagnetic field imposed by the transmitted fast electrons.

Successful examples using VEELS to measure semiconductor bandgaps have been demonstrated [1], which, in principle, envisage a sub-nm detection precision guaranteed by the ideal probe size of TEM. Nevertheless, besides the aberrations of the objective-lens system, delocalization of inelastic scattering can impose a significant effect upon the attainable spatial resolution, especially at very low energy losses. A rough estimation (based on a single atom calculation) of the inelastic delocalization length parameter d_{50}, within which 50% of the total delocalized intensity is confined, suggests that at an energy loss of 2 eV with an incoming energy of 200 keV for the fast electrons, d_{50} exceeds 10 nm. Under simplified assumptions, a universal expression can be developed as:

$$d_{50} \approx 0.6\lambda / \overline{\theta} \approx 0.5\lambda / \theta_E^{3/4},$$

where λ is the electron wavelength, $\overline{\theta}$ is the median angle of inelastic scattering, and θ_E is the characteristic scattering angle. Thus a large delocalization length is usually expected for small energy losses [2,3].

Figure 1 demonstrates a bandgap mapping using an $Al_{45}Ga_{55}N$/GaN/ sapphire structure with detailed experimental setup described in Ref. [2]. From the intermediate bandgap energies of about 3.7 eV close to the interface one might conclude that the bandgap transition between $Al_{45}Ga_{55}N$ and GaN is not abrupt. However, this apparent gradual change of the bandgap can mainly be attributed to the inelastic delocalization arising from the low energy losses involved. Note that a thin layer on the surface with a bandgap value of about 3.5 eV was detected as a mixed result of the presence of a glue line and inelastic delocalization.

By adopting an off-axis collection geometry, however, the situation can be improved. Figure 2 shows an EF-STEM micrograph of the same structure integrated

over the energy-loss range from 2.5 to 6 eV. Despite that the deduced band-gap map is noisy due to the narrow monochromator slit, a restricted energy selection range and the dark-field acquisition; after integration over a large region, i.e. 100×100 nm^2, the difference between the GaN and $Al_{45}Ga_{55}N$ band-gap onsets can be readily observed with enhanced spatial resolution. The results, however, are yet approaching atomic-level bandgap measurement which requires further sacrifice of the signal to noise ratio and possible involvement of the thermal diffused scattering at even larger collection angles.

References:

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[3] L. Gu et al., Ultramicroscopy 109 (2009) 1164.

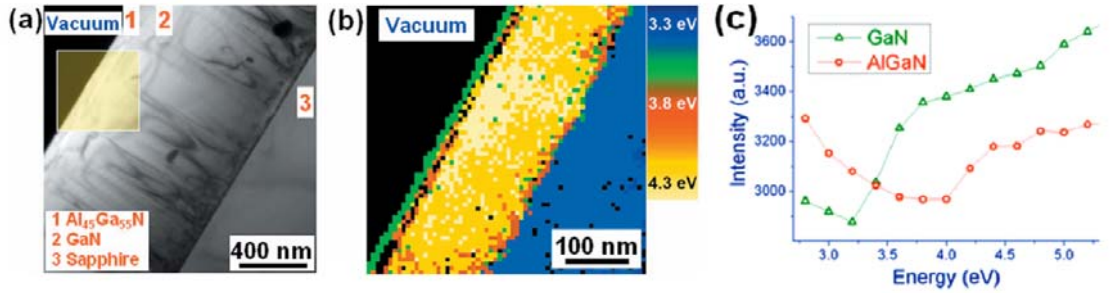

FIG. 1. (a) The sum of all energy-filtered images from 2 to 32 eV shows the $Al_{45}Ga_{55}N$/GaN/ sapphire structure. (b) Bandgap map of the region marked in (a) with a pixel size of about 7.2 nm, corresponding bandgap values can be read from the legend. (c) Electron energy-loss spectra extracted from the 3D EFTEM stack indicating a bandgap difference of about 0.8 eV. [2].

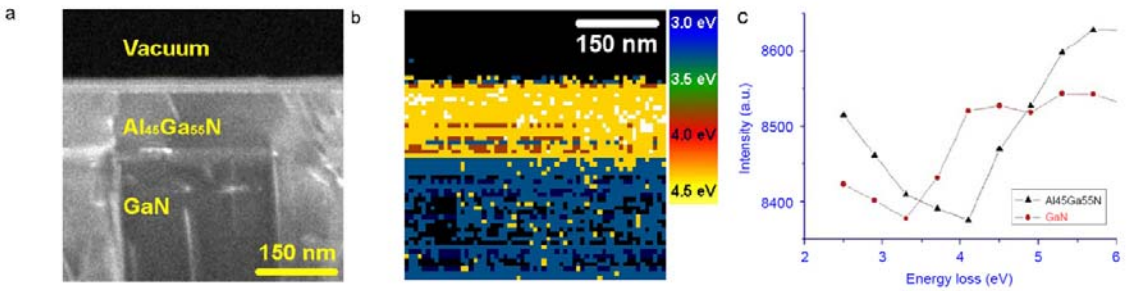

FIG. 2. Band-gap mapping of the same $Al_{45}Ga_{55}N$/GaN structure. (a) A raw EF-STEM micrograph integrated from 2.5 to 6 eV. (b) Band-gap mapping with the corresponding energy labeled on the right. (c) Extracted spectrum profiles of $Al_{45}Ga_{55}N$ and GaN. Detailed experimental procedure is described in Ref. [3].