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EELS Measurements on Wurtzite InN

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Recent successes in the growth of high quality wurtzite InN[1] have stimulated interest in the use of InN for high performance high electron mobility transistors (HEMTS) or light-emitting diodes.[2] However, unlike other III-V nitrides such as GaN or AlN, there is a dearth of reliable data on the basic structural, electronic and optical parameters and properties of InN.

Electron energy loss spectroscopy (EELS) is a powerful technique to measure some of these properties. Here we report EELS measurements on wurtzite InN using the Cornell UHV VG HB501 scanning transmission electron microscope (STEM) with a 100 keV electron beam and compare these with theoretical band structure calculations relevant to the observations.

The excitations of the N *1s* core-level electrons to the empty N *2p* states of conduction band give rise to the characteristic N K-edge spectrum in EELS which is presented in Fig. 1 where the positions of featuring peaks are identified. The dashed line (Fig. 1) is the calculated (using density functional theory within the local density approximation) N *2p* partial density of states in the conduction band of the InN. There is excellent agreement here on the relative position of the peaks. For In $M_{4,5}$-edge three broad peaks, P_1-P_3 at about 472 eV, 479 eV and 488-490 eV, are identified. The results of X-ray photoemission spectroscopy measurements[3] suggest that the primary contributions here in EELS come from transitions of the electrons from In $3d_{3/2}$ and $3d_{5/2}$ states to the corresponding In *5p* empty states of conduction band. In a simple model, we convolved the spectrum of the In $3d_{3/2}$ and $3d_{5/2}$ states (see Fig. 2(b)) with the calculated partial, In *5p*, conduction band DOS (Fig. 2(c)) which explains the presence of peaks P_1-P_3.

The next step was the study of the low-loss region of the EELS in InN. After Fourier-Log deconvolutions, the resulting single inelastic scattering distribution (SSD) is presented in Fig. 3. The strong peak located at 15.5±0.1 eV corresponds to this plasmon-loss. Calculations of the band structure predicts, as in the case of GaN, the presence of well-defined In *4d* deep valence states in InN. Photoelectronic spectroscopy measurements[3] carried out in InN confirms the existence of In *4d* states in InN. In low-loss EELS an inelastic interaction of the beam electrons with electrons of In *4d* states causes transitions of the latter into unoccupied states of the conduction band where the dipole selection rule eliminates all transitions except those into In *5p* empty states. Calculated In *5p* partial DOS of the conduction band convoluted with a simple Gaussian function for *4d* states is also presented in Fig. 3 (dashed line). The first peak of the DOS curve is aligned with peak A at 20.4±0.1 eV. As can be seen it describes the existence of peaks A-C in low-loss EELS (the broad peaks B and C are located within 23-25 and 34-40 eV ranges respectively). This predicts that, if we take into account the 1.9 eV band gap of InN, the In *4d* valence states are located 14.4±0.5 eV below the top of the valence band.[4]

Refereces

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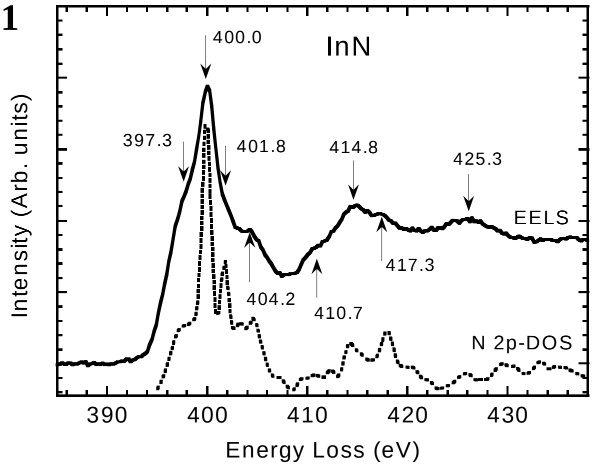

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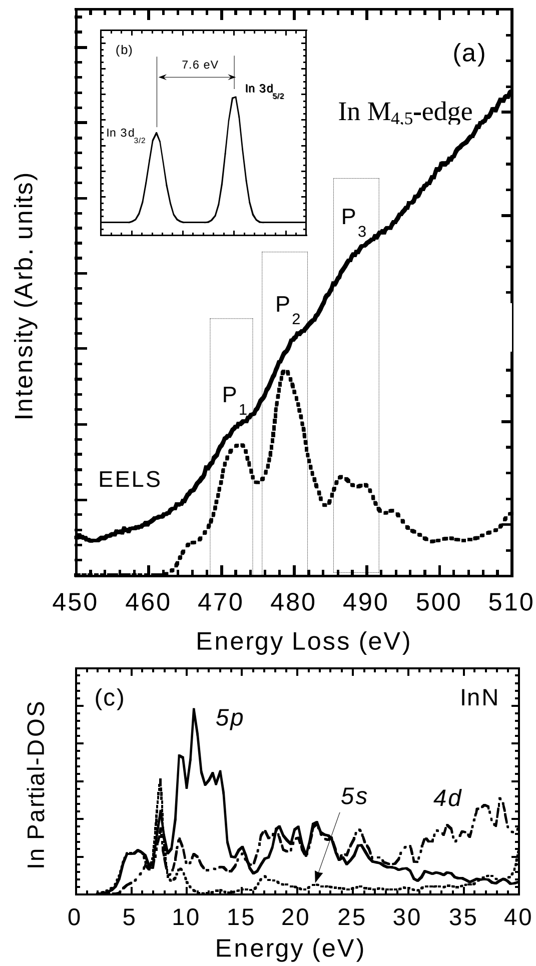

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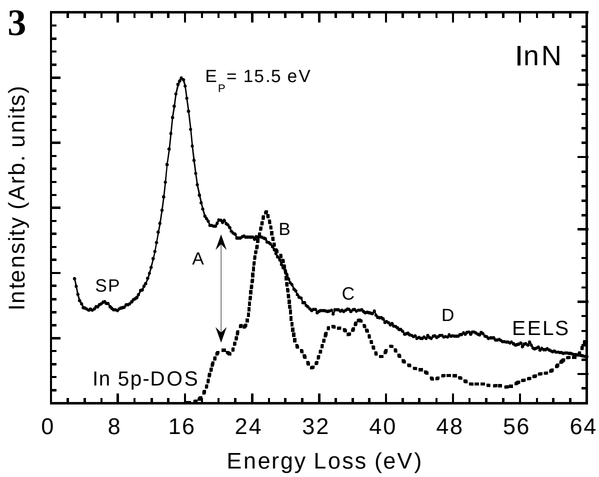

Fig. 1. Nitrogen *K*-edge from EELS measurements in wurtzite InN (solid line) with calculated nitrogen N *2p* partial DOS (dashed line). The DOS calculations are aligned to EELS by displacing the primary peak to 400.0 eV for better comparison of the remaining features.

Fig. 2. In $M_{4,5}$-edge from EELS measurements in wurtzite InN (solid line) with its theoretical prediction (dashed line) obtained by convoluting In $3d_{3/2}$ and $3d_{5/2}$ states (from Ref. 3) (b) with corresponding In *5p* empty conduction band DOS. (c) partial, In *5s*, *5p* and *4d*, DOS of the conduction band.

Fig. 3. Single scattering distribution obtained from low-loss EELS. The dashed line is calculated In *5p* partial DOS of the conduction band convoluted with In *4d* valence states.