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Monte Carlo Simulation of Electron Energy Loss Spectra of Group III-Nitride Nanoscale Semiconductors

M. Attarian Shandiz[1], F. Salvat[2] and R. Gauvin[1]

[1]Department of Materials Engineering, McGill University, Montreal, Canada.
[2]Facultat de Fisica (ECM), Universitat de Barcelona, Barcelona, Spain.

Group III-nitride semiconductors are a main research interest in the optoelectronics because of their unique physical and electronic properties [1]. The thin layers of these semiconductors at the nanoscale are now very common in the modern devices. Hence, proper materials characterizations with high spatial and compositional resolution such as electron energy loss spectroscopy (EELS) are essential for their research [2]. Monte Carlo (MC) simulation of EELS can provide useful information about the parameters of experimental EELS to obtain the best quantitative analysis. Optical data models have been proved as a proper physical model in MC simulations of EELS [3]. In the optical data models, the optical oscillator strength (OOS) is the main input for the calculations of inelastic scatterings [3].

In this research, the OOSs were built by the combination of optical properties resulted from density functional theory (DFT) calculations for the low-loss energy excitations and X-ray photoelectric data [4] for the core-loss excitations. Bethe sum rule was used to check the consistency of obtained OOSs. For the low-loss excitations, DFT calculations or available experimental data of the optical results related to the energy loss function (ELF) can be used. Figure 1a shows the DFT calculation results for the ELF of AlN, GaN and InN with wurtzite crystal structure performed by WIEN2k code [5]. New modified Becke-Johnson (mBJ) and local density approximation (LDA) were used as exchange and correlation potential for DFT calculations, respectively. Modified Becke-Johnson exchange potential leads to accurate band gap and electronic band structure for the semiconductors and insulators [6]. After obtaining OOSs, using the proper extension algorithms for the generalization of OOS, the inelastic cross sections for the MC simulation can be calculated. The LEEPS code [7] was adapted to perform MC simulation of EELS spectra. Figure 1b compares the simulated EELS for AlN, GaN and InN at the same conditions. The simulation provides the spectrum for the plasmon excitations at low-loss region as well as the core-loss excitations at high-loss region at the same time.

Several simulations for AlN, GaN and InN thin films at the same beam energy or the same thickness were performed to study their effect on the signal-to-noise ratio (SNR) as presented in Figure 2. The SNR was defined as $SNR=(I_{max}-I_{min})/(2I_{min})^{1/2}$, where I_{max} and I_{min} are the intensities above and below the ionization edge. Figure 2 shows the results for the calculation of SNR for N K edge. From the simulation results in Figure 2a, it can be inferred there is an optimum thickness for the SNR. Hence, to get the highest amount of SNR at the certain amount of beam energy MC simulation predicts a proper thickness. Figure 2b illustrates the results of the calculated SNR at the same thickness but at different beam energies. As it can be seen, by increasing the beam energy the SNR increases continuously. However, at very low beam energies for GaN and InN the amount of SNR is not considerable which can be improved by using higher amount of probe current or acquisition time. In the all simulations, N K edge in AlN provides higher SNR in comparison with GaN and InN at the same conditions. This can be explained by the less amount of average energy loss because of the lower atomic mass of AlN.
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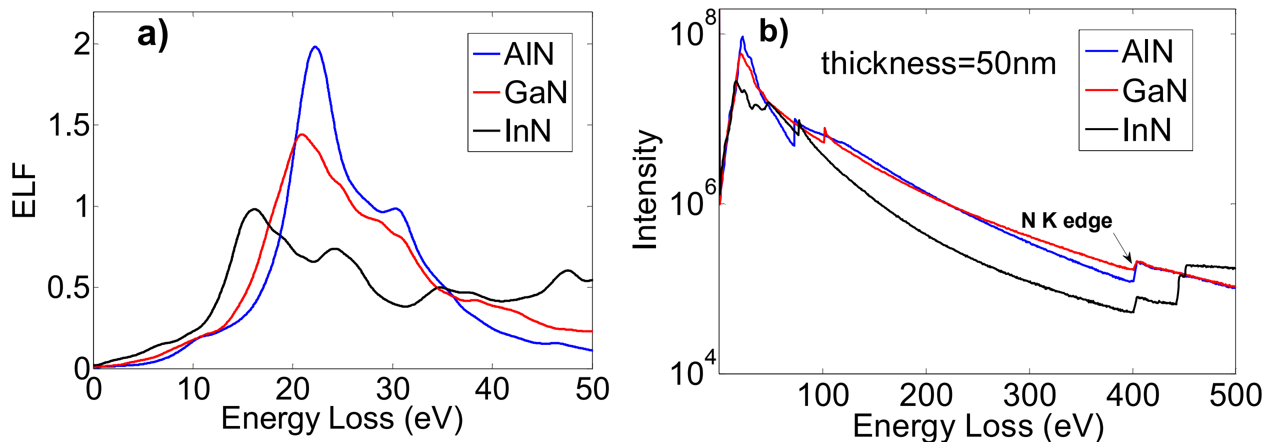

Figure 1. a) Energyloss functions (ELF) of AlN, GaN and InN in xx direction calculated by density functional theory calculations. b) Electron energy loss spectra of AlN, GaN and InN at the beam energy of 200 keV and the thickness of 50 nm.

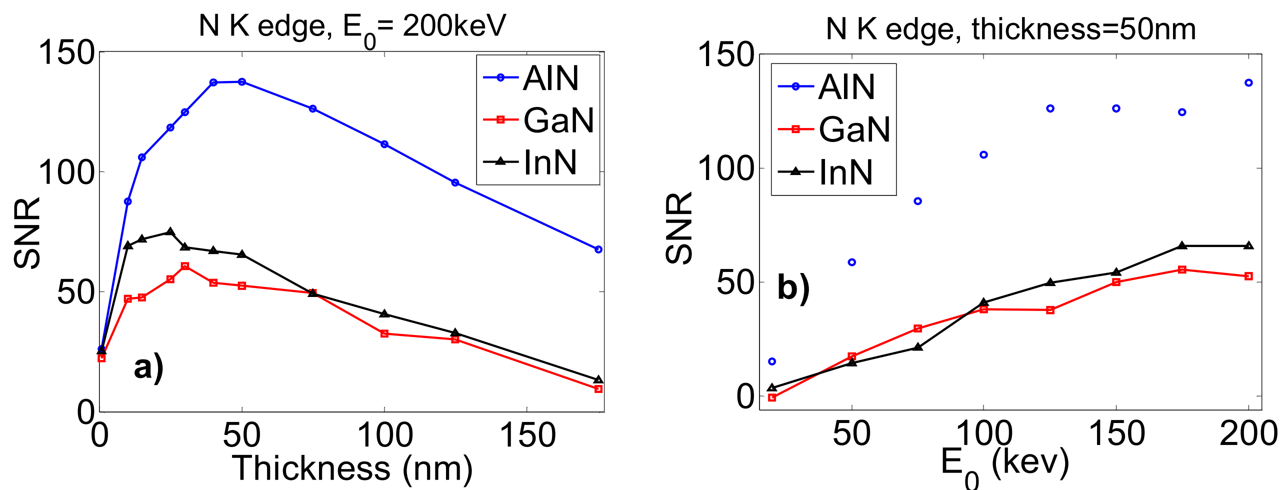

Figure 2. Signal to noise ratio of N K edge at a) the beam energy (E_0) of 200 keV and b) the 50 nm thickness. For the all EELS simulations, the probe illumination and collection angles were 5 and 10 mradin the simulations, respectively. Also, the spectrum acquisition time and the probe current were set to 1 s and 2 nA, respectively.

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