Application of the equation of motion method for the determination of the EXAFS Debye-Waller factors

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One of the puzzling parameters in the analysis of EXAFS spectra is the Debye-Waller factor (DWF) that accounts for the static and thermal disorder. In hexagonal semiconductors, e.g. GaN, the epitaxial growth of thin films as well as growth along non-polar orientations, result in strain-induced distortions of the nearest neighbor distances. The reliability and accuracy of the assessment of such distortions is increased drastically if the DWFs can be estimated independently by an appropriate method. Here we use the equation of motion (EM) subroutine of the FEFF8 package to calculate the DWFs and then to simulate the Ga-K-edge EXAFS spectra of GaN epilayers. The parameters used were the *a* and *c* lattice constants, as determined by XRD. The best values for the stretching force constants for the Ga-N, N-N and Ga-Ga interactions were found equal to 115, 38 and 23 N/m, respectively. These values reproduce very satisfactorily the Raman vibrational density of states (VDOS) as shown in Fig. 1. We point out that the Raman spectrum of the ion-implanted GaN is analogous to the VDOS due to relaxation of the selection rules. The contribution to the VDOS of the particular photoelectron scattering paths, depicted in the inset, is shown in the bottom panel of Fig.1. In Fig. 2 the experimental EXAFS spectra of an *a*-plane sample recorded at near-normal and near-grazing incidence are plotted along with the simulations in the k- and R-space.

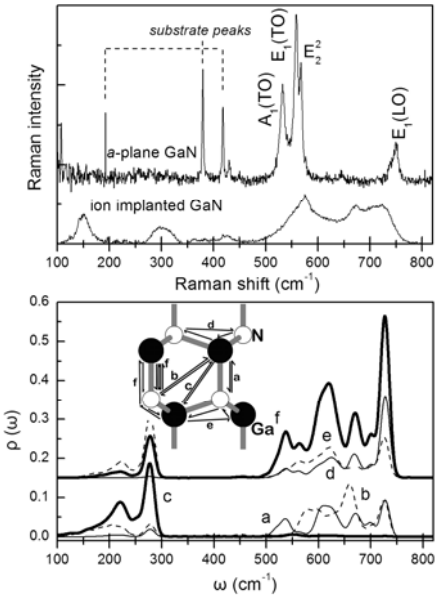

Figure 1: (top) Raman spectra of a crystalline- (*a*-plane) and a highly defective - (ion-implanted) GaN sample (bottom) Vibrational density of states of single (a,b,c), double (e,d) and triple (f) scattering paths indicated in the inset.

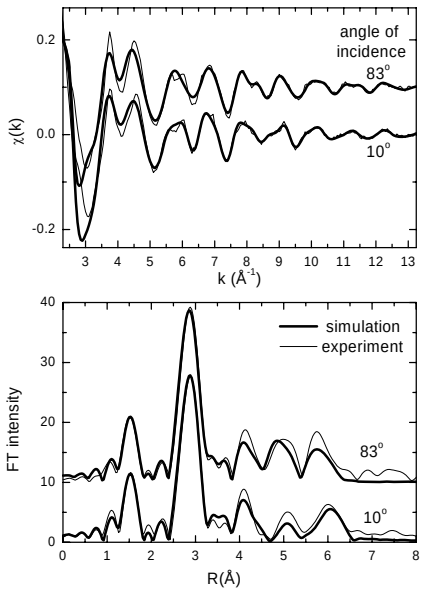

Figure 2: (top) χ(k) and (bottom) Fourier Transform amplitude of Ga-K-edge EXAFS spectra of an *a*-plane GaN sample for near-normal (83°) and near-grazing (10°) incidence. The *c*-axis was lying on the polarization plane of the synchrotron beam.

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