AlGaN multilayer examined by low-loss EELS and relativistic Kramers-Kronig analysis

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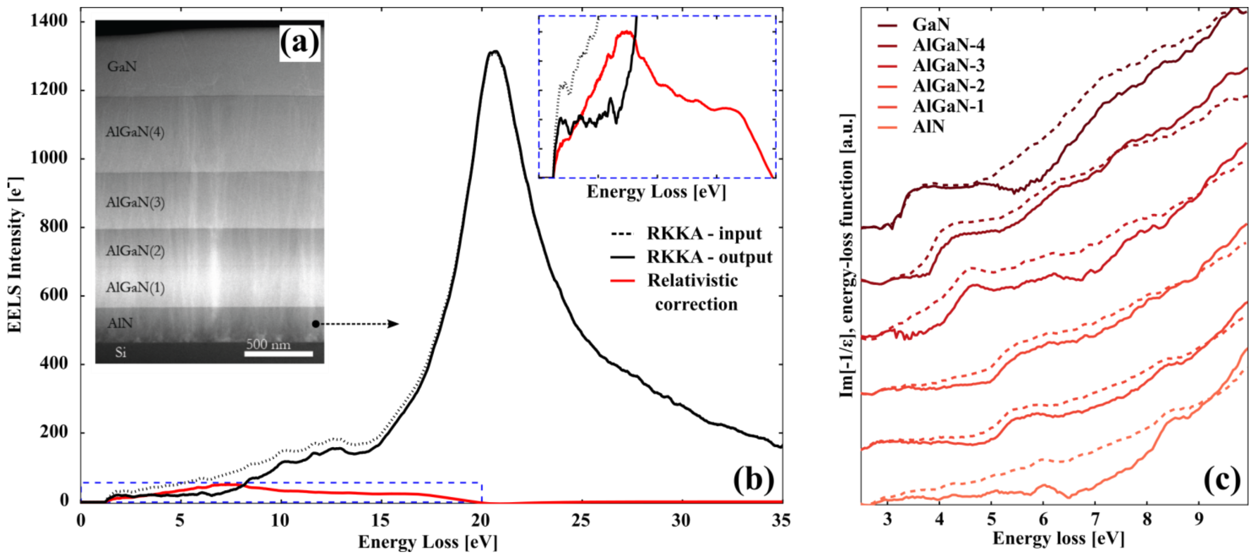
The relativistic losses affecting low-loss EELS may become relevant in cases when the speed of the transmitted electrons surpasses that of light in the material, $R(\mathcal{E}) > c^2/v^2$, and Cherenkov radiation may be emitted; for instance, on experiments carried out at higher voltages and/or in samples with a strong dielectric response. In dielectrics and semiconductors, the spurious EELS spectral features associated with relativistic effects impact the lowest energy-loss range, affecting signals in the band gap region. Indeed, this corruption might cause that other relevant spectral features are altered and not measured correctly and that, moreover, Kramers-Kronig analysis (KKA) may no longer be performed reliably. Nevertheless, a full-relativistic formulation of inelastic scattering including retarded fields is able to model these experiments. The somewhat more complicated dependencies in this model difficult directly normalizing the measured spectra and obtaining a correspondence with the dielectric function, $\varepsilon=\varepsilon(E)$, complicating purely full-relativistic alternative to the traditional KKA algorithm.

In this contribution a new KKA algorithm is presented, that is based on traditional KKA but takes into account relativistic losses (as proposed by Stöger-Pollach et al. *Ultramicroscopy* **108**, 439, 2008). Like in traditional KKA, this algorithm uses the non-retarded formulation to obtain ε from the input EELS data. From this result, a correction is calculated as the difference between the retarded and non-retarded predicted inelastic scattering distributions. This correction is then applied to the original input EELS data and the process is iterated. Our tests with synthetic data and a lamellar geometry indicate this algorithm has the ability to converge to a correct result for both ε and the relativistic correction in typically less than 10 iterations. In this sense, the algorithm can be used as a deconvolution procedure for relativistic losses.

In order to further test the performance of this algorithm, it has been employed in the analysis of an experimental EELS dataset obtained from an AlGaN multilayer sample. This sample features relatively large layers, see panel (a) in the included Figure, with different uniform alloy compositions covering the whole compositional range. The experimental conditions (monochromated FEI-Titan STEM operated at 300 kV) and the thickness of the sample in some of the studied regions, preclude the analysis of the spectra at energy-loss range below ~ 10 eV without considering relativistic losses. In particular, the low energy-loss range in the thick pure AlN regions, see panel (b) and inset, is impacted by Cherenkov losses modifying the shape of the measured signal. The relativistic KKA algorithm is used to calculate a correction to the measured spectrum, revealing a band gap edge close to the expected 6.2 eV for AlN. The composition and thickness of each layer is also measured using standard low-loss EELS methods such as Plasmon peak characterization. With this information and using a linear model for the compositional dependence of the refractive index of the alloy, relativistic KKA can be applied to the spectra acquired in the sample as portrayed in panel (c). The results of this procedure allow us to study the whole energy range of these low-loss EELS spectra.



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