Determining alloy concentration by analyzing dynamic diffraction at strained semiconductor interfaces

Frederik Otto[1], Dr. Laura Niermann[1], Dr. Tore Niermann[1], Prof. Dr. Michael Lehmann[1]
[1]Technische Universität Berlin, Berlin, Germany

Background incl. aims

In the realm of semiconductor devices, particularly in the context of quantum well lasers, the optical properties are shaped by bandgaps and band offsets derived from precisely engineered alloy concentrations in ternary semiconductors, exemplified by InGaAs quantum wells in GaAs. While S/TEM possesses the necessary spatial resolution for resolving sharp interfaces, EDX typically lacks precision in determining the alloy concentration. However, during epitaxial growth on a substrate, lattice mismatch induces stress at the interface, resulting in localized lattice deformations known as strain. When preparing a thin transmission electron microscopy (TEM) lamella of a strained interface, the stress supporting this strain lacks support on the top and bottom of the lamella, leading to stress relaxation. For a compressively strained layer, this corresponds to the lamella bulging outwards at the interface. The magnitude of this relaxation is unique to the strain at the interface cause by the lattice mismatch, and hence by the alloy concentration in the layer.

The aim of this study is to deduce the alloy concentration of compressively strained InGaAs quantum wells in a GaAs matrix through a detailed analysis of stress relaxation at the lamella's surfaces. This is accomplished by evaluating patterns inside the diffraction discs using scanning convergent electron beam diffraction (SCBED). These patterns, manifestations of multiple electron scattering or dynamic diffraction, exhibit high sensitivity to small changes in displacement in electron beam direction and consequently, to stress relaxation at the lamella’s surfaces. Alloy concentrations are determined by matching beam simulations of relaxed lamellas with varying parameters to the experimental data.

Methods

We prepare a TEM-lamella containing InGaAs layers with known In-concentration in GaAs close to the [100] zone axis using FIB. Deriving information involves detailed reproduction of measured features through simulations to infer the original lamella state. For computational efficiency, we tilt specimen along a quantum well layer into [002] systematic row conditions. Full 2D diffraction patterns (256x256 pixels) are recorded at each scan position within a 256x256 scan window. The resulting 4D dataset can be reduced to a 2D-representation, named as x-q plot, by considering the problem’s symmetry. This reduction involves focusing on one spatial coordinate x orthogonal to the layer. Additionally, only one reciprocal coordinate q along the systematic row, into which the specimen was tilted, is considered. The convergence angle is chosen to achieve non-overlapping discs.

To model the experimental data in simulations, we employ a two-step forward calculation process: Initially, we model the initial stress and the resulting relaxation by doing finite element calculations, providing the layer width, elastic constants and lattice mismatch as inputs. The resulting displacement is then incorporated into beam simulations, numerically propagating the Darwin-Howie-Wheelan (DHW) equation. The simulations are fine-tuned to align with experimental conditions, accounting for tilt, specimen bending, and lamella thickness.

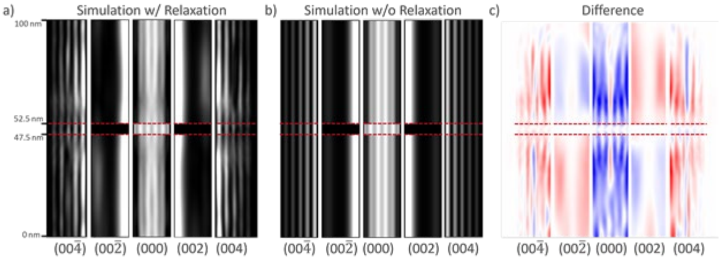
Results

Leaveraging the nominal alloy concentration of a 5 nm wide In0.23Ga0.77As quantum well within GaAs, we successfully replicate dynamic diffraction features in simulations, yielding three key outcomes, as illustrated in Fig. 1. Firstly, our measurement reveals distinct features discernible in the x-q plot, unveiling changes in dynamic diffraction, even at considerable distances of multiple quantum well widths from the interface (Fig. 1 a). Secondly, comparing these findings with DHW beam simulations that omit surface relaxation highlights the absence of these long-ranging features, conclusively attributing them to surface relaxation (Fig. 1 b, c). Lastly, by manipulating the initial lamella alloy concentration, we can modulate the influence of surface relaxation. Minimizing the discrepancy between the measurement and simulations for the Indium concentration allows us to faithfully reproduce the nominal Indium concentration. These results are validated using STEM-EDX and dark-field imaging of a chemically sensitive reflection. We further discuss the method's limitations concerning specimen thickness, quantum well width, and alloy concentration.

Conclusion

Our study successfully identifies the nominal alloy concentration of a compressively strained InGaAs quantum wells in GaAs through a detailed analysis of stress relaxation at the TEM-lamellas surfaces. This accomplishment involves precisely replicating dynamic diffraction features within diffraction discs through simulations. These simulations account for surface relaxation by incorporating the displacement from finite-element calculations of the strained interface for a given specimen thickness. The process of minimizing discrepancies between measurement and simulation by adjusting the alloy concentration opens a novel avenue of discerning semiconductor alloy concentrations at strained interfaces by analyzing the impact of surface relaxation on dynamic diffraction.

Graphic:



Keywords:

Strain, Relaxation, composition-determination, dynamic-diffraction, 4D-STEM