Analyzing Dynamic Diffraction at Strained Semiconductor Interfaces: A Method to Determine Alloy Concentrations

Frederik Otto*, K. Jakob, R. Specht, L. Niermann, T. Niermann, M. Lehmann

Technische Universität Berlin, Strasse des 17. Juni 135, 10623 Berlin, Germany

*Corresponding author: frederik.otto@tu-berlin.de

Four-dimensional scanning transmission electron microscopy (4D-STEM) allows for the acquisition of full 2D electron diffraction patterns at each scan position of a focused electron probe and therefore allows for investigation of strain at the interfaces of semiconductor materials with high spatial resolution. However, achieving electron transparency requires thinning TEM lamellae to just a few tens of nanometers. This thinning process results in the absence of atoms at the lamella’s surfaces, which can lead to surface strain relaxation in pseudomorphically grown materials. Specifically, for tensile-strained layers, this relaxation causes the TEM lamella to effectively collapse inward at the interface, resulting in local deformation. This deformation affects multiple electron scattering, appearing as patterns within the diffraction discs, a phenomenon known as dynamic diffraction.

While conventional strain measurements in S/TEM aim to minimize the impact of these dynamic diffraction effects, we adopt a different approach - we choose to directly evaluate features of dynamic diffraction as indicators of TEM lamella surface relaxation. Our method involves comparing experimental diffraction patterns to simulations generated through a two-step forward calculation process. First, we model the lamella in its relaxed state by solving the elasticity problem using finite-element calculations. The resulting displacement fields are then used as input for Darwin-Howie-Whelan calculations to simulate the patterns of dynamic diffraction.

Our experimental data matches the simulations closely, and we demonstrate that the degree of relaxation depends on the alloy concentration within the strained layer. By minimizing the differences between experimental measurements and corresponding simulations, we propose a method to reconstruct the alloy concentration in semiconductor layers based on the initial stress at the interface and known substrate properties.