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Dynamical X-ray Diffraction from $In_xGa_{1-x}As$ Heterostructures with Dislocations

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High-resolution x-ray diffraction is an important nondestructive tool for structural characterization of semiconductor heterostructures, and the diffraction intensity profiles contain information on the depth profiles of strain, composition, and defect densities in device heterostructures. Much of this information remains inaccessible because the lack of phase information prevents direct inversion of the rocking curves. The current practice is to use dynamical simulations in conjunction with a curve-fitting procedure to indirectly extract the profiles of strain and composition, but such dynamical simulations have been based on perfect, dislocation-free laminar crystals, which renders the analysis inapplicable to highly mismatched structures containing dislocation densities greater than about 10^6 cm^{-2}. In this work we present a dynamical model for Bragg x-ray diffraction in semiconductor device structures with nonuniform composition, strain, and dislocation density, which is based on the Takagi–Taupin equation for distorted crystals and accounts for the diffuse scattering arising from the strain mosaicity and angular mosaicity associated with dislocations. We show theoretically that the x-ray diffraction profiles from $In_xGa_{1-x}As$/GaAs (001) heterostructures are strongly affected by the depth distribution of the dislocation density as well as the composition and strain, so that in principle all three distributions may be obtained by the analysis of the measured diffraction profiles.

Key words: X-ray diffraction, metamorphic heterostructures, InGaAs, dislocations, dynamical diffraction

INTRODUCTION

High-resolution x-ray diffraction measurements allow determination of depth profiles of strain, composition, and defect densities in device structures. Dynamical[1–6] and kinematical[7–11] simulations have been used in conjunction with a curve-fitting procedure to extract the profiles of strain and composition, but are based on perfect, dislocation-free laminar crystals, which renders the analysis inapplicable to mismatched structures with dislocation densities greater than 10^6 cm^{-2}. Krivoglaz and Ryaboshapka[12] and Levine and Thomson[13] have analyzed the line profiles of Bragg peaks from crystals containing straight, parallel screw dislocations with precisely known atomic displacements. Though their treatment is mathematically rigorous, it is not possible to determine all of the atomic displacements in a real crystal containing a dislocation network with a diversity of dislocation orientations, shapes, and Burgers vectors. For this reason we consider the ensemble of dislocations in a defected semiconductor heterostructure to be described by characteristic distributions associated with the ensemble-average angular and strain broadening of the Bragg profiles by the dislocations. This approach is quite general, but for its application here we have considered the specific case of Gaussian distributions to calculate the Bragg diffraction profiles from semiconductor structures with nonuniform strain, composition, and dislocation density. Because it has been shown in previous work that curve fitting to dynamical simulations allows the extraction of the strain profiles in semiconductor heterostructures, we focused on the dislocation density and composition profiles in this research. Therefore, to simplify their interpretation,

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