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Effect of Epilayer Tilt on Dynamical X-ray Diffraction from Uniform Heterostructures with Asymmetric Dislocation Densities

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In this work we extend the dynamical theory of Bragg x-ray diffraction to account for a tilted, asymmetrically defected, uniform-composition epitaxial layer atop a (001) substrate. In a zincblende semiconductor there are eight active slip systems, within which two distinct types of dislocations exist. These two types are distinguished by their misfit segments, which are oriented along either the [110] or [$1\bar{1}0$] direction. The two threading dislocation densities can be measured by observing the variation of the x-ray rocking curve width with the incident beam azimuth. However, the tilting of the epilayer also has a measurable and potentially conflicting effect on the rocking curve as a function of azimuth. First, the peak position varies by (nominally) twice the layer's absolute tilt within a full azimuthal rotation. Second, the tilting of the layer affects the epilayer rocking curve width. Through use of the modified dynamical diffraction theory, we show that the peak width's azimuthal dependence on tilt is of only second order, so that the layer misorientation with respect to the substrate need not be considered for the purpose of determining the two dislocation populations by x-ray diffraction. Dynamical simulations were performed and compared with experimental measurements for a ZnSe/GaAs(001) structure grown by photoassisted metalorganic vapor-phase epitaxy, and in this way the two dislocation density populations were found to be $D_A = 1.6 \times 10^8$ cm^{-2} and $D_B = 2.0 \times 10^8$ cm^{-2}.

Key words: x-ray diffraction, dynamical theory, ZnSe, HgCdTe, dislocations, epitaxial layer tilt, asymmetric dislocation densities

INTRODUCTION

Dynamical x-ray diffraction (XRD) simulations[1–6] are currently used with a curve-fitting procedure to obtain composition and strain depth profiles in semiconductor device structures. However, these simulations are based on perfect crystals, which renders the analysis inapplicable to structures having dislocation densities higher than 10^6 cm^{-2}. In recent work,[7] we developed a technique to model defected heterostructures. In this model, the two ways in which dislocations distort the lattice are taken into account: mosaic block angular variation and interplanar spacing variation. Here, we have improved upon this model to differentiate between α- and β-type dislocations. One can determine the two populations separately by making multiple XRD measurements at different azimuths, and comparing the rocking curves with simulations.

THEORY

Dynamical Diffraction from Perfect Crystals

Dynamical diffraction from a zincblende crystal is described by the Takagi–Taupin equation[1–3]

$$-i\frac{\mathrm{d}X}{\mathrm{d}T} = X^2 - 2\eta X + 1, \qquad (1)$$

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