STRAINS AND MISFIT DISLOCATIONS AT INTERFACES

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INTRODUCTION

In recent years there have been great advances in the heteroepitaxial growth of non-lattice-matched epilayers and strained-layer superlattices (SLSs). The role of lattice strain in these structures is extremely important. Not only does strain exert a large influence on band gaps, band offsets, effective masses and mobilities, but strain can be used deliberately to "fine-tune" these device properties. Hence it is essential to be able to measure local strains in order to understand and quantify the physical properties of the material. In this paper we will illustrate the use of Convergent Beam Electron Diffraction (CBED) for the measurement of local strain, and we will describe the use of a new technique, Convergent Beam Imaging (CBIM), for detecting, mapping and measuring small crystalline distortions.

As is well known, in very thin strained epilayers, the epilayer-substrate strain is initially accommodated elastically, but at sufficiently large epilayer thicknesses misfit dislocations occur at or near the substrate-epilayer interface. These dislocations, and particularly the threading dislocations connecting the misfit dislocations to the growth surface, can seriously affect the electrical properties of the epilayer and it is therefore important to minimise their density. The process by which misfit dislocations are first introduced when the substrate is dislocation free has been the subject of debate for a number of years. In this paper we will describe a new internal dislocation source we have called the diamond defect: a single diamond defect can act as a regenerative source of misfit dislocations which propagate to lie in an orthogonal array at the interface.

MEASURING LOCAL STRAINS BY CBED

It is well known that Higher-Order Line Zone (HOLZ) lines in the bright-field disc of CBED patterns can provide accurate measurements of lattice parameters to within about 1 part in 104, with about 40 Å spatial resolution. This has been used by the authors to detect and measure local strains in Si/Ge\textsubscript{x}Si\textsubscript{1-x} SLSs, and other materials\textsuperscript{2,3,4}.

We shall illustrate the application of CBED with reference to investigations of a model Si/Ge\textsubscript{x}Si\textsubscript{1-x} strained-layer structure (with growth direction [100]) which is shown in fig.1. The structure was grown by molecular-beam epitaxy: for details of the growth conditions see refs 2 and 5. (001) cross-sections of this Si/Ge\textsubscript{x}Si\textsubscript{1-x} SLS were used and [001] zone-axis CBED patterns recorded. This orientation has the great advantage that deviations from cubic symmetry are immediately visually apparent in the CBED patterns.
Fig. 1. Bright-field cross-sectional image of a Si/Ge\textsubscript{x}Si\textsubscript{1-x} strained-layer structure which shows from left to right the following: Si(100) substrate; Si buffer 0.1 μm thick; Ge\textsubscript{0.05}Si\textsubscript{0.95} alloy 1 μm thick; Si buffer 1 μm thick; Ge\textsubscript{0.10}Si\textsubscript{0.90} alloy 1 μm thick. The electron beam direction is approximately [011] and the crystal growth direction is [100] which is parallel to the [400] g vector used for imaging. Each interface is identified by arrowheads.

Fig. 2 shows a typical CBED pattern from the Si substrate, from which it is obvious that the pattern symmetry is 4mm (i.e. a fourfold axis, namely [001], with two independent sets of mirror planes), as expected for a cubic crystal. Fig. 3 shows a pattern from a Ge\textsubscript{x}Si\textsubscript{1-x} epitaxial layer, where \(x\) is at 5%. It is clear that the material is not cubic, and the pattern has symmetry 2mm, which is consistent with a tetragonal structure. However, detailed computer simulation shows that the HOLZ pattern observed in fig. 3 cannot be accounted for by a tetragonal distortion along the [100] growth direction. If variable values not only of \(a_{100}\) (growth direction) but also of \(a_{001}\) (to allow for surface relaxation) are considered, then excellent computer matches to experiment are obtained. Hence the effects of surface relaxation are to give a structure which is, in general, orthorhombic. The experimental values of the distortion thus obtained lie between those expected for a bulk crystal and a fully relaxed crystal\textsuperscript{4}.

DETECTING MONOCLINIC FORMS OF Ge\textsubscript{x}Si\textsubscript{1-x}

Fig. 3 was recorded from a region of Ge\textsubscript{0.05}Si\textsubscript{0.95} away from the Si/Ge\textsubscript{0.05}Si\textsubscript{0.95} interface. CBED patterns recorded closer to the interface show a breakdown of the mirror planes present in fig. 3, implying a monoclinic structure. The patterns from 10% Ge-Si are even clearer in their loss of mirror symmetry, see fig. 4, and in this case the break in mirror symmetry is observed independent of the distance from the heterointerface.

There are two possible sources for the symmetry breaking exhibited in fig. 4. First, the substrate orientation may not be precisely (100): vicinal (100) substrates off-cut towards, say, either (011) or (010) should give monoclinic epilayers. Second, if the cross-sectional sample deviates from a perfect (001) orientation this may cause symmetry breaking since the strain relaxation occurs along the specimen normal: this latter effect appears to dominate in our case since some residual symmetry breaking is apparent from a detailed examination of CBED patterns from the Si substrate, close to the interface.

The above results may be of considerable significance since they demonstrate that materials which in their bulk form may be, say, cubic (e.g. bulk Ge\textsubscript{x}Si\textsubscript{1-x} alloy) may become tetragonal, orthorhombic or monoclinic under "strain engineering" deliberately using surface