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Structural and electrical non-uniformities in thin CdTe layers grown on InSb by MBE

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Abstract. Electrical measurements made on CdTe layers grown on (001) InSb substrates reveal significant non-uniformities as a function of depth. As there is a small mismatch between the lattice constants for CdTe and InSb, extended defects resulting from strain relief in the epilayer are believed to have an important influence on the electrical properties and, with the aid of computer modelling to simulate x-ray diffraction rocking curves, the distribution of structural defects is being explored. Examples are presented of carrier concentration depth profiles in the vicinity of the CdTe–InSb interface for samples grown under a variety of different conditions and the relationship between the observed electrical non-uniformity and the distribution of dislocations resulting from strain relief is discussed.

1. Introduction

Due to the device potential of the magneto-optical and magneto-transport properties of a variety of II–VI based semiconductor materials containing magnetic ions, much consideration is currently being given to the controlled growth of these materials as single films or multilayer structures. In this laboratory, attention has been concentrated on low-dimensional structures, involving the $Cd_xMn_{1-x}Te$ system, grown by MBE on (001) InSb substrates. In the course of studies aimed at improving our understanding and control over the properties of these structures, interest has developed in some non-uniformities observed in the electrical properties of thin single layers of the materials. Such layers were previously reported to be n-type without deliberate doping and it was assumed that this was due to In donors being incorporated as a result of diffusion from the underlying substrate [1]. However, the results of more recent studies reported in this paper show that, although the free carrier concentration is usually not uniform within a layer, the variation with depth is not consistent with that which would result from In diffusion. Indeed, instead of an expected reduction in carrier concentration with increasing distance from the substrate, the reverse is frequently observed.

In seeking an explanation for the observed non-uniformities in the electrical properties of these layers, consideration has been given to the possible structural non-uniformities which might arise from the relief of strain in the layer associated with the small mismatch between the lattice constants for the epilayer and the InSb substrate. From the analysis of x-ray diffraction rocking curves and the employment of computer simulation techniques, the experimental results are shown to be consistent with the existence of a non-uniform strain structure within the epilayers, with most of the strain relief occurring within a very thin region close to the substrate. The influence of different growth conditions and the associated effects on the electrical properties are discussed.

2. Experimental details

The MBE system employed for the growth of the layers was a VG Semicon V80H system with pyrolytic boron nitride Knudsen cell crucibles. The Cd and Te components were provided by a single source of high purity CdTe (from MCP Ltd) but additional Cd was available from a further Cd cell and there were additional separate sources of Mn and In. The substrates were 0.5 mm thick wafers of (001) InSb (obtained from MCP Ltd) and the epilayer growth rate was usually about 0.7 μm h^{-1} at substrate temperatures in the region 240–250 °C.

After polishing and etching, the substrates were mounted on a molybdenum plate using Ga–In solder and after evacuating the system, the surface oxides were removed by argon ion etching followed by thermal annealing to remove the ion damage. Several etch/anneal cycles were normally required before a clear 2×4 RHEED pattern, characteristic of a clean InSb surface, was obtained.

Double crystal x-ray diffraction (DCXRD) rocking curves were obtained to provide information about the lattice structure of the epilayers and, with the aid of a computer model constructed using the dynamical theory of x-ray diffraction, their structural uniformity. Information on the electrical properties was deduced from capacitance–voltage measurements made on Schottky barriers formed by evaporation of a gold contact onto the epilayer surface or by contact with an electrolyte. Using the latter, in conjunction with a Polaron Profiler, controlled electrochemical etching could be employed to strip material from the epilayer surface, in known increments, in order to construct a profile of the electrical properties as a function of depth. In order to check that the observed variations with depth were not associated with the profiling method, some samples were studied using a combination of these two techniques. For example, after a part of a profile had been established using electrochemical etching, a sample was removed from the electrolyte and, after providing a gold contact, a conventional C–V measurement was made. Consistent results were always obtained.

3. Results and discussion

As has been previously reported [1], undoped CdTe and CdMnTe layers grown on InSb tend to be n-type and this has been attributed to the incorporation of In from the substrate during growth. However, the free carrier concentrations in these undoped layers is usually less than 10^{15} cm^{-3} and for thin epilayers the Schottky barrier depletion layer width can exceed the epilayer thickness (usually less than 2 μm), so that no depth profile of the properties can be obtained. For samples with free carrier concentrations at the upper end of the observed range, depth profiles are possible and these frequently reveal significant non-uniformity, as for the example shown in figure 1. For this sample, a drop in carrier concentration of more than one order of magnitude is observed, from about 5×10^{15} cm^{-3} close to the surface to about 10^{14} cm^{-3} in the vicinity of the substrate. It is clear that this variation cannot be attributed to a non-uniform distribution of In due to diffusion from the InSb substrate, for which the concentration gradient would be opposite to that in figure 1. Indeed, it is now clear from work on deliberately doped samples that the observed variation in carrier concentration cannot be due to a non-uniform distribution of impurities. For example, figure 2 shows the profile for a layer which was grown in the presence of a steady In flux to yield uniform In doping at a level in excess of 10^{16} cm^{-3}. The form of the resultant profile seen in figure 2 is clearly very similar to that for the undoped sample in figure 1 apart from a rather abrupt variation in the rate of change of the gradient at approximately 0.9 μm from the surface. It should be noted that, in addition to the doping, the sample in figure 2 was grown with two very thin (50 Å wide) MnTe barrier layers mid-way through sample and this could be responsible for the discontinuity in the profile gradient, but this has yet to be confirmed by growing layers with similar barrier structures at different depths.

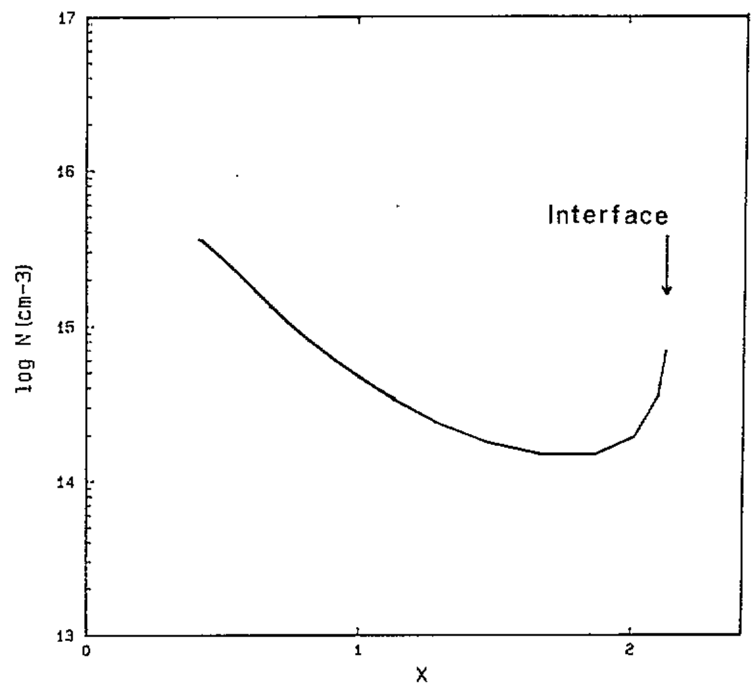

Figure 1. Carrier concentration N as a function of depth x (in μm) from surface for an undoped CdTe layer.

As for the case shown in figure 2, it is generally found that, for 2 μm thick samples, the free carrier concentration approaches a near uniform level, consistent with the incorporated donor density, in the region close to the surface and falls gradually further below the donor state density at greater depths. This same behaviour is observed in samples which are non-uniformly doped as well as in the previously discussed uniformly doped cases. For example, figure 3 shows the profile for a sample consisting of three layers, of approximately 0.7 μm each, with the In concentration increasing in steps from approximately 2×10^{17} cm^{-3} in the surface layer, to approximately 3×10^{18} cm^{-3} in the layer closest to the substrate. In a previous reference to a similarly constructed sample [1], attention was drawn to the apparent reduction in activation efficiency of

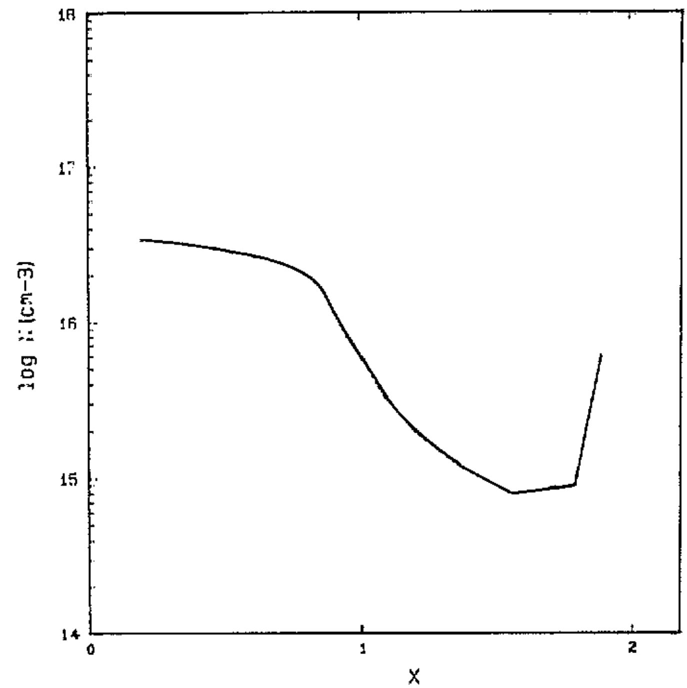

Figure 2. Carrier concentration N as a function of depth x from surface for a uniformly doped CdTe layer.

the donor atoms as the concentration increased to higher values. However, it can also be seen in figure 3 that, within each region of uniform In concentration, the variation in carrier concentration follows the pattern obtained for the less heavily doped sample of figure 2. Following a fairly uniform region close to the surface, there is a slight downward movement towards the edge of the top layer; the gradient increases significantly in the second layer and diminishes in the third.

In view of the consistent form of the carrier concentration profile for samples of different type, both undoped and heavily doped, it seems unlikely that diffused impurities play an important role. However, it is possible that structural defects could be responsible. As there is a small mismatch between the lattice constants for CdTe and InSb (0.05%), dislocations and other extended defects resulting from the relief of strain in the epilayer are expected to be generated in the vicinity of the substrate–epilayer interface. Such effects lead to a broadening of the peaks in the DCXRD rocking curve, a typical example of which is shown in figure 4 for a 2 μm thick CdTe sample. From the angular separation between the dominant (CdTe) peak and the smaller (InSb) peak, it is concluded that the epilayer is nearly commensurate with the substrate but it is clear from this figure that the CdTe peak is not quite symmetric, as should be the case for a single, uniform layer. This peak is broadened towards angles of greater separation from the InSb peak indicating that part of the CdTe layer exists in a superstrained state. As described previously [2], a computer model has been constructed to simulate the rocking curves for a variety of different single and multilayer structures. This model, employing the dynamical theory of x-ray diffraction, provides a satisfactory fit to the curve in figure 4 if it is assumed that the superstrained region lies at the interface, with most of the excess strain being

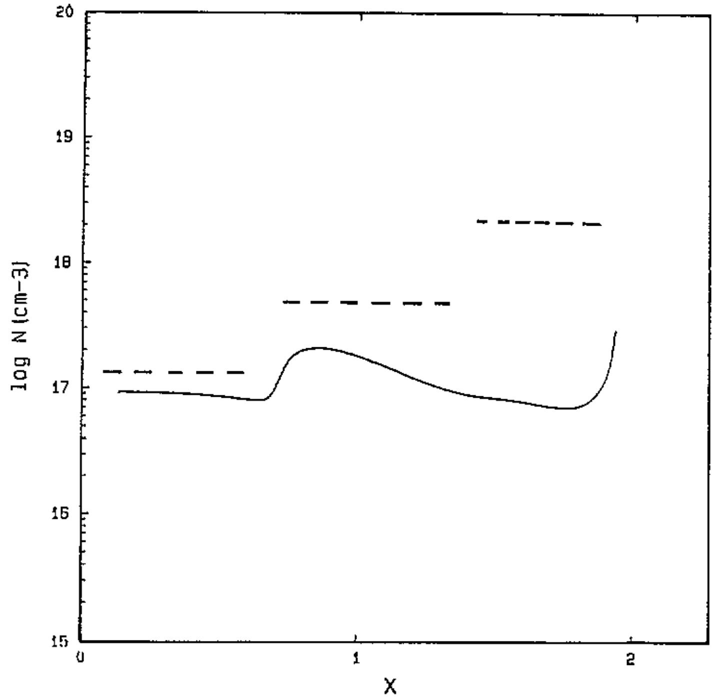

Figure 3. Carrier concentration (full curve) and In concentration as determined by SIMS measurements (broken line) for a non-uniformly doped CdTe layer.

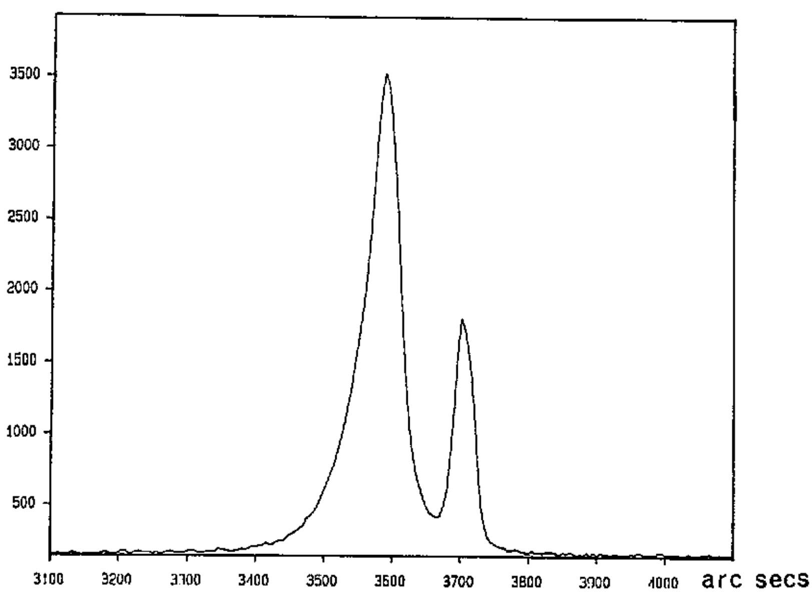

Figure 4. A Cu Kα (004) double crystal XRD rocking curve for a 2 μm thick CdTe layer on a (001) InSb substrate.

gradually relaxed over a distance of 0.5 μm.

Dislocations resulting from lattice relaxation can be expected to act as sinks for

In atoms, making them electrically inactive or as sources of Cd vacancies, generating acceptor states to compensate the active donors. Either mechanism would lead to a reduced carrier concentration in the vicinity of the epilayer–substrate interface, as observed, but examination of samples grown under non-stoichiometric conditions indicates that cadmium vacancy generation might play the dominant role. Growth with an excess Cd flux (which would be expected to inhibit Cd vacancy formation) has been shown to yield much improved uniformity in the carrier concentration in both doped and undoped samples [2]. It is believed [3–5] that Cd vacancy formation can also be suppressed by growth under laser illumination (photo-assisted MBE or PAMBE) whereby the Cd/Te atomic ratio at the growth surface is increased by laser-induced desorption of Te [6]. Such a mechanism is consistent with the suggestion by Golding *et al* [7] that the residence time of Cd atoms on the growth surface is less than that of Te so that the use of a stoichiometric flux tends to yield excess surface Te which can interact with the InSb substrate to form an In_2Te_3 interfacial layer. With a lattice constant of 6.158 Å (much less than that of InSb) such a layer could be responsible for the additional strain in the CdTe layers discussed earlier, but this has yet to be confirmed.

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