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Deep Level Transient Spectroscopic Investigations of Boron Doped Si and Si/$Si_{1-x}Ge_x$/Si Layers Grown by MBE

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This work reports deep level distributions in Si/$Si_{1-x}Ge_x$/Si layers as determined via Deep Level Transient Spectroscopy (DLTS). Well defined states observed in the Si capping layer are attributed to dislocation-point defect interactions. Varying degrees of broadening observed in the spectra - to a lesser extent in the Si capping layer whilst much more pronounced in the first heterojunction region and $Si_{1-x}Ge_x$ layer - may be considered either in terms of trap emission over a band of energies or as a consequence of the significant band bending which occurs at the heterojunction.

This work follows on from our previously reported direct assessment of the Si/Si_{1-x}Ge heterojunction via Capacitance-Voltage (C-V) measurements [1, 2]. Details of MBE growth and Schottky contacts used for the depletion capacitance measurements are given elsewhere [1]. A narrow 1V window (of fill duration 3ms) was used to allow the broadened features to be resolved and to profile the bulk Si, $Si_{1-x}Ge_x$ and heterointerfacial regions for a variety of Ge compositions.

Typical deep level spectra for a p-doped 10^{16} cm^{-3} Si/$Si_{0.88}Ge_{0.12}$/Si structure are shown in Fig.1. Whilst well defined peaks are observed in the Si cap, considerable distortion is seen as the depletion edge moves into the vicinity of the first heterojunction - the distortion attributed to the heterojunction lies in the reverse bias regime -6 to -11V. As the depletion edge is extended into the bulk $Si_{0.88}Ge_{0.12}$ region away from the first heterojunction, the distortion is somewhat reduced and peaks start to be resolved. Fig.2 shows the apparent trap distributions as determined via an approach adopted by Hawkins [4] - note trap activations are energetic displacements from the valence band edge. Whilst no discernible trends with increasing Ge composition were observed in the distorted deep level spectra in the vicinity of the first heterojunction, apparent trap concentrations were observed to increase with increasing Ge composition in the alloy layer. The well defined states A, B, C and D in the Si capping layer all exhibited logarithmic filling behaviour and no meaningful value for capture cross-section could be obtained.

C-V measurements indicated the bulk trap distribution to be compensating centres ie. donor-like. The absence of the Poole-Frenkel effect [4] and the observed logarithmic filling behaviour [5] further verify this. Observation of non-exponential transients was investigated using simulations based on the work of Omling *et al.* [6]; such behaviour has been interpreted in terms of trap emission from a band of deep level energies [6, 7]. This allowed the degree of broadening of the well defined peaks in the bulk regions to be determined; however, the applicability of this model in accounting for the gross distortion observed in the vicinity of the first heterojunction requires care. It is more probable that such effects will be observed as a consequence of the significant band bending in this region and cannot be attributed to this band of deep levels alone; the possible origins of such distortion lie with the valence band offset, interface charge density and interfacial misfit dislocations [8] although the latter is considered to have a minimal role. Trap profiling in the vicinity of such band bending can become questionable: apparent trap activation energies may vary as a consequence of trap emission to valence band edges where the energetic displacement is spatially dependent and a particular deep level may cross the Fermi level at more than one point, broadening the deep level spectra and making its extracted spatial position inaccurate. Furthermore, interface charge or the build-up of coulomb potentials on dislocation-related states can change the occupancy of deep levels such that DLTS may not detect all the electrically active states present.

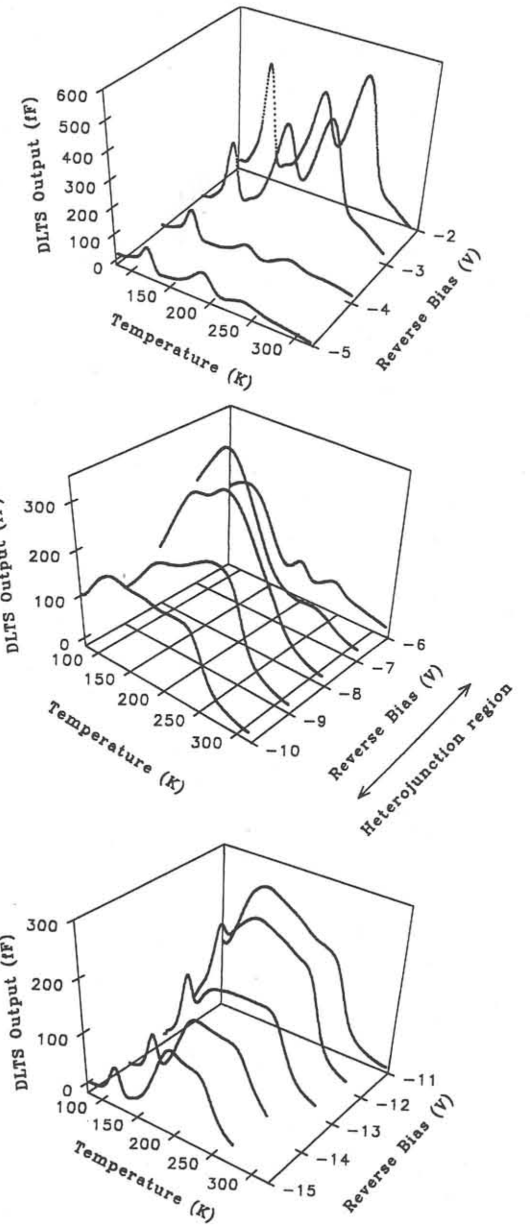

Fig 1. Deep level spectra profiling through the $Si/Si_{0.88}Ge_{0.12}/Si$ structure.

The origins of the observed electrical activity is most probably a complex interaction between a variety of sources; some comments may be made in the light of structural analysis. Increasing s-pit densities, as determined via defect etch /Nomarski techniques for samples grown at higher temperature or samples subjected to short anneals, corresponded to reduced electrical activity as observed via DLTS. This suggested removal of metallics from a point defect form into electrically inactive precipitates [9]. Threading dislocation densities remained unchanged. No significant misfit dislocation densities were apparent from defect etch/Nomarski techniques, indicating the strained integrity of the layers despite their thickness exceeding the equilibrium critical

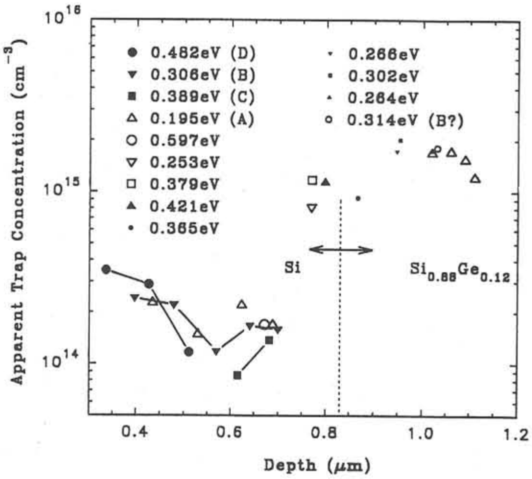

Fig 2. Apparent trap distributions for the $Si/Si_{0.88}Ge_{0.12}/Si$ structure.

thickness. Previous reports have indicated dislocation-point defect interactions can result in donor-like states [10] and so produce energy bands [11] similar to observations made here. Furthermore, Transmission Electron Microscopy (TEM) indicated the presence of Fe located preferentially in the alloy layer, which suggested the strain inherent in the alloy layer was acting as an effective sink for metallics; this contamination has since been identified as most likely originating from the elemental Ge charge used in MBE growth. There was also evidence of compositional banding similar to the observations made by Fraser *et al.* [12]; such compositional banding may produce variation in the band structure, resulting in the moderate broadening of features observed in the alloy.

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