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(G*) Experimental analysis of surface Debye temperature for epitaxial thin films

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Defect engineering plays an essential role in materials science and is of paramount importance in thin-film device fabrication. Novel experimental methods are needed to identify and quantify defects during film growth. The Debye temperature (DT) of a solid is a representation of the stiffness and so is sensitive to defect concentrations. The DT tends to decrease in the vicinity of the surface such that the endpoint value found for the top atomic layer is known as the surface DT. In this collaborative project, we have used a suite of surface characterization techniques to characterize and quantify defects on the surface and in the near-surface region in epi-films compared to single crystals. We applied Rutherford Backscattering Spectroscopy (RBS, random and channeling modes), Positron Annihilation Spectroscopy (PAS), and Low Energy Electron Diffraction (LEED) to study defect density and distribution and calculate surface DT for different epitaxially grown thin films (Si films on sapphire, and Ge on Si (001)). We used Rutherford Backscattering Spectroscopy (RBS) in a channeling alignment to measure defect distribution as a function of depth, which can be correlated with PAS measurements, giving information about defect densities. These results were compared with surface DT calculated from LEED patterns which showed that the larger the concentration of defects in the epitaxial layer, the lower is the surface DT. For example, the surface DT's of bulk Si (001), 1μm Si on sapphire, and 0.6μm Si on sapphire were 609K, 574K, and 535K, respectively. However, experimental uncertainties of LEED DT are large and show dependence on the diffraction peak index, electron energy, and inner potential in calculations. Overall, we found good agreement between estimates of surface DT from LEED, defect densities estimate from RBS, and PAS results.

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