Dislocation Mediated Corrugation of Ge-Si (001) Interface

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Interfaces play a key role in determining the electrical and thermal transport properties of semiconductor devices. To investigate the effect of dislocations on the structuring of the Ge-Si (001) interface, transmission electron microscopy characterization was performed on epitaxial Ge thin films deposited on (001) Si using molecular beam epitaxy. This heteroepitaxial system promotes the formation of misfit dislocations at the interface due to the over 4.2% lattice parameter mismatch between Si and Ge at growth and annealing temperatures. Samples are characterized both before and after annealing at 800 °C for 10 minutes. Dislocations promote interdiffusion at the interface through their surrounding stress field and by serving as vacancy sinks, which can result in corrugation of the interface at certain growth or annealing temperatures. Lomer dislocation climb in epitaxial Ge on Si (001) has previously been simulated to operate through a vacancy mediated process [1]. As dislocations sink vacancies to climb, a counter flux of atomic species diffuses away from the dislocation core, strongly preferring Ge due to its elevated diffusivity across most of the $Si_{1-x}Ge_x$ compositional range [2]. Edge dislocations additionally exert a stress field near the interface, creating a stress gradient that promotes Ge diffusion into the substrate. These combined effects, the exerted stress gradient and vacancy sinking, promote corrugation of the interface. Cross section transmission electron microscopy images show initially ordered arrays of misfit dislocations along the interface in an as-grown sample that are observed to climb after annealing, motivated by diffusion induced stress as Ge more rapidly diffuses into the substrate. High angle annular dark field scanning transmission electron microscopy images reveal interface structuring and movement before and after annealing. The initial corrugation seen in the as-grown sample evidences the dislocation mediated structuring of the interface, as the diffusivity of the atomic species at the growth temperature is too low to account for the observed diffusion lengths. Deeper corrugations are observed after dislocations climbed during the annealing process, further reinforcing the suggested mechanisms of interface structuring. High resolution annular dark field scanning transmission electron microscopy shows the corrugation as a contrast difference between the brighter Ge and darker Si. Simulations were performed using a Euler forward march to iteratively solve equations governing the diffusion process in the presence of stress gradients and ideal vacancy sinks [3]. The simulated concentration profiles agree with the observed magnitude of corrugation after a 10 minute anneal at 800 °C, further supporting the role played by misfit dislocations in structuring the interface.

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