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Quantitative Correlations of Stress Field and Threading Dislocation Configurations in Si/Si_{1-x}Ge_x/Si(100) Strained Layers CHI-CHIN WU, Virginia Military Institute, ROBERT HULL, Rensselaer Polytechnic Institute — The equilibrium configurations of the threading dislocation connecting misfit dislocation dipoles in Si/Si_{1-x}Ge_x/Si(100) heterostructures have been analyzed by simulation, and compared to experimental images to investigate the correlations of stress field variations and dislocation configuration in capped heteroepitaxial thin films. Calculations are based on the energy equations for dislocations in elastically isotropic crystals over all possible dislocation angular configurations, and the orientations with the minimum total energy are determined as functions of the magnitude and variations of the film stresses. It is determined that the configuration with the misfit dislocation leading at the cap/film interface (as opposed to the film/substrate interface) is increasingly favored either with increasing magnitude of local film stress/strain or with the variation in calculated geometry of the threading dislocation.

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