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Dislocations in $Ge/Si_{1-x}Ge_x$ films: atomistic simulations and elastic-theory calculations FRANCESCO MONTALENTI, ANNA MARZEGALLI, LEO MIGLIO, INFM and LNESS, Materials Science Department, University of Milano-Bicocca, Via Cozzi 53, 20125 Milano (Italy) — Molecular dynamics simulations based on Tersoff potentials are used to investigate 60° dislocation stability and mobility in compressed Ge films on $Si_{1-x}Ge_x$ [1]. For low misfit values glide dislocations appear as partials (90° and 30°), separated by a stacking fault. By increasing the misfit, dissociation is no longer observed, and the core geometry becomes the perfect, Hornstra one. Elastic-theory calculations provide an explanation of the observed behavior, caused by the stress- dependent effective force acting on the two cores. Shuffle dislocations, on the other hand, behave very differently. Under high compressive strain conditions, indeed, the perfect Hornstra core is conserved during the fast gliding motion observed in the simulations. The above described misfit-dependent behavior is consistent with recent experimental results [2]. [1] A. Marzegalli, F. Montalenti, and Leo Miglio, Appl. Phys. Lett. (in press). [2] D. Chrastina et al., Thin Solid Films 459, 37 (2004).

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