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Equilibrium shape and dislocation nucleation in strained epitaxial nanoislands J. JALKANEN, Helsinki University of Technology, Finland, O. TRUSHIN, Institute of Microelectronics and Informatics, Russia, K. ELDER, Oakland University, E. GRANATO, Instituto Nacional de Pesquisas Espaciais, SP Brasil, T. ALA-NISSILÄ, Helsinki University of Technology, Finland, S.-C. YING, Brown University — We study numerically the equilibrium shapes, shape transitions and dislocation nucleation of small strained epitaxial islands with a two-dimensional atomistic model, using simple pair potentials [1]. We first map out the phase diagram for equilibrium island shapes as a function of island size and lattice misfit with the substrate. When the interactomic potential minimum depth ϵ is the same for substrate and adsorbate, the latter either wets the surface or has one of three generic equilibrium island shapes. As ϵ favours substrate-adsorbate interface, Stranski-Krastanow growth mode emerges between complete wetting and island formation zones while in the opposite case the islanding zone is extended. A simulation based extrapolation scheme predicts an optimal island shape for attractive ϵ. The energy barriers and transition paths between different island shapes and dislocation nucleation in initially coherent islands are investigated with Nudged Elastic Band method. We also discuss the elastic behaviour of these systems in terms of the Phase Field Crystal model [2]. [1] J. Jalkanen, O. Trushin, E. Granato, S. C. Ying, and T. Ala-Nissila, Phys. Rev. B 72, 081403 (2005) [2] K. Elder and M. Grant, Phys. Rev. E **70**, 051605 (2004)

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