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Atomic mechanisms of misfit dislocation nucleation in Pd/Cu and Cu/Pd heterostructures OLEG TRUSHIN, Institute of Microelectronics and Informatics RAS, Russia, TAPIO ALA-NISSILA, Helsinki Institute of Physics and Laboratory of Physics, Helsinki University of Technology, Finland, ENZO GRANATO, Laboratorio Associado de Sensores e Materiais, Instituto Nacional de Pesquisas Espaciais, Brasil, SEE-CHEN YING, Department of Physics, Brown University — Generation of misfit dislocations during growth of heteroepitaxial films is a long standing problem in technology. Effective control of the relaxation processes in such systems requires understanding atomic mechanisms of defect formation. Pd/Cu and Cu/Pd systems (with misfit value about 7%) represent typical model systems to study this problem. We used molecular static simulations with EAM potential and extensive saddle point search methods to estimate energetics and find possible transition paths for strain relaxation processes in these systems. FCC(111) and FCC(100) lattice structures were considered. Different transition paths for strain relaxation , which lead to formation of defects of different types were investigated. Systematic study of the process as function of film thickness was performed. We revealed strong asymmetry between compressive and tensile strain cases, which is due to asymmetry of repulsive and attractive parts of the interatomic potential.

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