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Stress release mechanisms for Cu on Pd(111) in the submonolayer and monolayer regimes GIULIA ROSSI, JARI JALKANEN, Helsinki University of Technology, Department of Applied Physics, Espoo, Finland, ENZO GRANATO, Laboratório Associado de Sensores e Materiais, Instituto Nacional de Pesquisas Espaciais, Sao José dos Campos, Brasil, OLEG TRUSHIN, Institute of Physics and Technology, Yaroslavl Branch, Academy of Sciences of Russia, Yaroslavl, Russia, SEE-CHEN YING, Department of Physics, Brown University, Providence, US, TAPIO ALA-NISSILA, Helsinki University of Technology, Department of Applied Physics, Espoo, Finland — Metallic surfaces and nanostructures are essential systems for heterogeneous catalysis. Cu on Pd(111) is an interesting system, with a large mismatch (-7.1 percent). We study strain relaxation mechanisms of Cu on Pd(111) up to the monolayer regime using two different computational methodologies, basin hopping global optimization and energy minimization with a repulsive bias potential. Our results are consistent with experimentally observed layer-by-layer growth mode. However, we find that the structure of the Cu layer is not fully pseudomorphic even at low coverages, but forms fcc and hcp stacking domains, separated by partial misfit dislocations. We estimate the minimum energy path and energy barriers for transitions from the epitaxial state to the fcc-hcp domain pattern. This work encourages further experimental investigations directly probing the overlayer structure.

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