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Ge islands ordering on top of multilayered Ge/Si structures: from atomistic data to AFM measurements FRANCESCO MONTALENTI, RICCARDO MARCHETTI, LEO MIGLIO, INFM and LNESS, Materials Science Department, University of Milano-Bicocca, Italy, GIOVANNI CAPELLINI, MONICA DE SETA, FLORESTANO EVANGELISTI, INFM and Physics Department, University of Roma Tre, Italy — The strain field induced by a buried Ge island in a Si capping layer (CL) is investigated by Tersoff-potential molecular dynamics simulations. It is shown that the tensile region above the island changes both quantitatively and qualitatively by increasing the thickness of the CL. A simple model based on thermodynamic arguments and on the local energetics predicted by the simulations shows that small Ge islands directly grown over the capping layer surface tend to arrange in flower-like shapes for a thin CL, while they cluster in a more close-packed way over a thick CL. A direct comparison with recent CVD-grown multilayered SiGe structures is carried out. The simulated minimum-energy shapes are shown to agree rather well with AFM images of the Ge-island distribution on top of the outermost layer.

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