Abstract Submitted
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Thermodynamic potentials in closed and open nanocrystalline systems: Si-Ge islands on Si(001). MARINA S. LEITE, Brazilian Synchrotron Light Source, Instituto de Fisica Gleb Wataghin - UNICAMP, ANGELO MALACHIAS, Max-Planck Insitute for Solid State Research, STEFAN W. KYCIA, University of Guelph, TED I. KAMINS, R. STANLEY WILLIAMS, Hewlett-Packard Laboratories, GILBERTO MEDEIROS-RIBEIRO, Hewlett-Packard Laboratories, Brazilian Synchrotron Light Source — The driving forces for alloying in Si-Ge epitaxial nanocrystalline islands were quantified experimentally. Closed and open systems were emulated by controlling surface diffusion kinetics [1]. Grazing Incidence X-Ray Diffraction (GIXRD) experiments were performed to map the composition and the strain distribution within the Si-Ge:Si(001) islands, permitting the evaluation of the relevant thermodynamic potentials for alloying. For the closed system the elastic strain energy increased, which was more than compensated by the increase in the local mixing entropy [2]. In contrast, for the open system, the elastic energy decreased and the mixing entropy increased, driven by the intermixing originated from the inflow of Si from the reservoir. For both systems, the evolution of the composition leads to a lowering of the Gibbs free energy. The results were in full agreement with a theoretical prediction of the optimum concentration for epitaxial islands. [1] M. S. Leite *et al*, Phys. Rev. Lett. **98**, 165901 (2007). [2] G. Medeiros-Ribeiro *et al*, Nano Lett. **7**, 223 (2007).

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