



ΓΕΝΙΚΟ ΣΕΜΙΝΑΡΙΟ ΤΜΗΜΑΤΟΣ ΦΥΣΙΚΗΣ

PHYSICS COLLOQUIUM

Thursday, 12 February 2015

17:00 -18:00

3rd Floor Seminar Room

“Interplay of Thermodynamics and Kinetics in the Nanoworld”

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Abstract

One of the longstanding issues in heteroepitaxy regards the origin and shape of composition profiles (CPs) in semiconductor nanoislands. This is important for the optoelectronic properties in device applications. A much debated issue is whether intermixing and alloying processes are driven by equilibrium thermodynamics or by non-equilibrium kinetic effects. A prototypical example is given by alloyed Ge nanoislands grown/embedded in Si, providing a very promising route for producing quantum dots. A fascinating effect recently observed [1] is atomic ordering in dome-shaped SiGe islands, in which the distribution of species, thinking in terms of bulk equilibrium, should be random.

In this talk, I will first discuss the fundamentals and review some key research on these issues. I will then present our recent atomistic Monte Carlo (MC) simulations [2] which explained the ordering effect in SiGe nanoislands, showing that ordering is a surface-related phenomenon driven by facet equilibrium than surface kinetics. Finally, I will present new results of MC simulations [3] showing that both thermodynamics and kinetics play a crucial role in the alloying process and the formation of CPs. The former is the driving force for alloying, while the latter controls it through the kinetic barriers of atomic diffusion in the system.

[1] A. Malachias *et al.*, Phys. Rev. B 72, 165315 (2005); Phys. Rev. B. 82, 035307 (2010); M. Richard *et al.*, Appl. Phys. Lett. 106, 012108 (2015). [2] G. Vantarakis, I. Remediakis, and P.C. Kelires. Phys. Rev. Lett. 108, 176102 (2012). [3] C. Georaiou, T. Leontiou, and P.