Universidad Carlos III de Madrid

Seminario del Instituto Gregorio Millán

Equations for step bunch formation in the morphological evolution of nano-scale crystal surface structures below the roughening transition

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Resumen

We derive "Lagrangian" coordinates continuum equations for the surface evolution, obtained as a limit from a nano-scale description of the dynamics ("discrete" step-interaction equations). At the nano-scale, below roughening, the crystal surface consists of arbitrarily shaped, interacting steps that move by diffusion of point defects (adatoms) on terraces; and attachment and detachment of adatoms at steps. The cases of diffusion-limited (DL) kinetics, attachment-detachment limited (ADL) kinetics, and mixed DL+ADL kinetics are considered, with the restriction of axial symmetry in the surface.

The standard ("Eulerian") continuum description fails when step bunching (where a relatively large number of steps coalesce to form "bunches" of very closely packed steps) occurs. A numerical investigation of the continuum Lagrangian equations for the ADL case shows that they capture step bunching — where the bunches appear as the product of the interaction between a (destabilizing) negative diffusion (arising from step-line tension effects) and a stabilizing fourth order nonlinear diffusion (arising from the step-step interactions). The local dynamics within each bunch can be described by a (relatively) simple equation — resembling, in some sense, the Kuramoto-Sivashinski equation — combining these two effects.

- DÍA: **Lunes 16 de marzo de 2009 (ATENCIÓN: DÍA INUSUAL)**
- HORA: **12:30**
- LUGAR: **Edificio Sabatini. Aula 2.1.D04**