

Structure and electronic states of vicinal noble metal surfaces with densely kinked steps

G. Vasseur¹, J. Lobo-Checa^{2,3}, I. Piquero-Zulaica², F. Schiller², T. Einstein⁴, J. E. Ortega^{1,2,5}

¹Donostia International Physics Center DIPC, San Sebastian, Spain

²Centro de Física de Materiales, CFM-CSIC, San Sebastian, Spain

³Instituto de Ciencia de Materiales de Aragón (ICMA), Universidad de Zaragoza, Spain

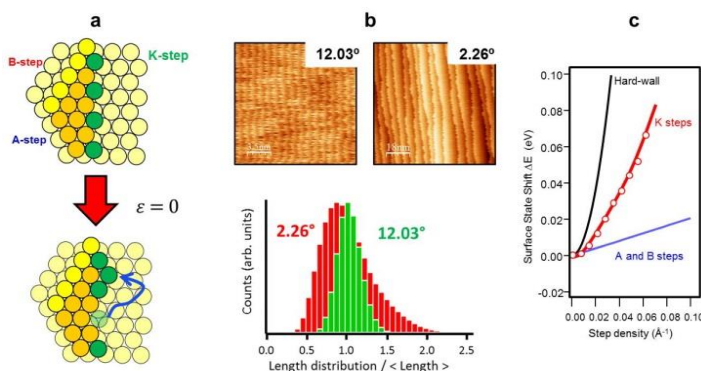
⁴Department of Physics, University of Maryland, College-Park, Maryland, USA

⁵Departamento de Física Aplicada I, Universidad del País Vasco, San Sebastian, Spain

E-mail: enrique.ortega@ehu.es

The thermal excitation of step-edge atoms into “kinks” ($e^{-\frac{\epsilon}{kT}}$) is the essence of the step dynamics on a crystal surface. At a vicinal surface with high step densities, kinks also influence the equilibrium shape at finite temperature. At $T=0$, the density of kinks strongly depends on the in-plane orientation of the surface. At fcc - (111) vicinal planes close-packed step-edges (A-type and B-type) run parallel to equivalent [1-10] directions. As shown in Fig. 1a, steps oriented along the [11-2] direction exhibit a “100% kinked” step-edge (K-type), where out-protruding step-edge atoms have no direct nearest-neighbors parallel to the step. Remarkably, as sketched in the same Fig. 1a, in such K-steps thermal excitations have zero energy cost $\epsilon=0$, allowing meandering and roughening of steps without energy penalty. Our objective is to investigate, theoretically and experimentally, the impact of this property in step dynamics, equilibrium shape, growth, and electronic states of K-stepped surfaces.

First experiments have been performed using a Ag single crystal curved around the (654) direction, which allows one to probe with STM and Angle Resolved Photoemission (ARPES) all K-type vicinal surfaces from the (111) plane up to $\alpha=18^\circ$. In Fig. 1b we show characteristic STM images and terrace-width distribution histograms for $\alpha=2.26^\circ$ and $\alpha=12.03^\circ$. A remarkably neat transformation is observed from low to high step-densities, suggesting a dramatic transition in step interactions, from purely entropic, at low step-densities, to strongly elastic, at high step-densities. In Fig. 1c we show the energy shift ΔE of the Shockley band measured with Angle Resolved Photoemission across the curved sample. Large ΔE values are found compared to close-packed steps, indicating strong repulsive scattering due to a larger electric dipole at K-type steps. The connection of these STM and ARPES results with the particular step energetics and dynamics of K-type vicinal surfaces will be discussed.



(a) Schematic description of atomic K-steps and the thermal excitation of step-edge atoms, with zero energy cost. (b) STM images (top) and terrace width distribution analysis (bottom) of two K-stepped surfaces. Experiments are performed on a curved Ag(654) crystal. (c) Surface state shift as a function of the step density, measured by ARPES on the Ag(654) curved crystal.