Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Thermal stability and diffusion of defects on an Al(100) FRANCESCA BALETTO, NICOLA MARZARI, DMSE-MIT — Understanding and controlling homoepitaxial metal-on-metal growth is a key challenge in surface physics due to its great technological interest. We use a combination of classical and ab-initio techniques, including molecular dynamics and transition-state finding, to identify the dominant mechanisms of diffusion for adatoms and vacancies on an Al(100) surface. We find that exchange and concerted exchange mechanisms, well known in adatom diffusion, play also a central role in vacancy diffusion. In addition, they lead to a distinct phase transition localized in the first layer as temperature is raised.

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Date submitted: 20 Nov 2006 Electronic form version 1.4