Abstract Submitted
for the MAR10 Meeting of
The American Physical Society

Gold on silicon: Structure and energetics of Si(111)-(5x2)-Au STEVEN ERWIN, Naval Research Laboratory, INGO BARKE, University of Rostock, Germany, F. J. HIMPSEL, University of Wisconsin-Madison — Gold forms linear chain-like reconstructions on several vicinal surfaces of silicon, as well as on Si(111). We propose a new structural model for Si(111)-(5x2)-Au that incorporates three Au chains per surface unit cell. Five main theoretical results, obtained from first-principles total-energy calculations, support the model. (1) In the presence of silicon adatoms the periodicity of the gold rows spontaneously doubles, in agreement with experiment. (2) The dependence of the surface energy on the adatom coverage indicates that a uniformly covered phase is unstable and will phase-separate into empty and covered regions, as observed experimentally. (3) Theoretical scanning tunneling microscopy images are in excellent agreement with experiment. (4) The calculated band structure is consistent with angle-resolved photoemission data. (5) The calculated activation barrier for diffusion of silicon adatoms along the row direction is in excellent agreement with the experimentally measured barrier. These results for the flat Si(111)-(5x2)-Au surface also shed light on the widely studied Au chain systems that form on the vicinal surfaces Si(557) and Si(553), as will be discussed. [1] S.C. Erwin, I. Barke, and F.J. Himpsel, Phys. Rev. B 80, 155409 (2009).

Steven Erwin
Naval Research Laboratory

Date submitted: 18 Nov 2009 Electronic form version 1.4