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Evidence of Copper Interstitials on Si(001) ARNALDO LARACUENTE, LANE BAKER, JAMES SULLIVAN, LLOYD WHITMAN, Naval Research Laboratory — We describe the surface structures following sub-monolayer Cu deposition on Si(001) and subsequent hydrogen termination as characterized by scanning tunneling microscopy. Cu adsorption at 870 K results in a characteristic (2×8) island+vacancy structure, as previously reported. After H-termination, the dominant features of the island+vacancy structure remain, but the size and distribution of the structures are significantly altered. Based on the atomic-scale appearance of both the clean and H-terminated structures, we propose that Cu absorbs through interstitial locations ejecting Si surface dimers in the process. Density functional theory of the potential energy surface for Cu adsorption on Si(001) is consistent with this model, predicting that absorption takes place primarily between dimers and dimer rows. Most of the near-surface Cu is underneath the Si islands and within the vacancies, with the remaining residual in interstitial sites. After H-termination of the Cu/Si(001), all the surface atoms are H-terminated Si, and all Cu is actually subsurface.

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