Stress Evolution During Monolayer Deposition of Cu on Au (111)

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The deposition of Cu on Au (111) follows the Stranski-Krastanov (SK) growth mode both in vacuum and electrolyte. The misfit for this system is -12.8%. In electrolytes the wetting layer is pseudomorphic and the deposition occurs on the bulk-terminated 1 x 1 Au (111) surface. Using bulk values of the elastic constants, a pseudomorphic Cu monolayer (ML) on Au (111) should yield a surface stress change (bulk coherency stress x thickness) of + 7.76 Jm^{-2}. In vacuum the pseudomorphic character of the wetting layer is ambiguous in that some of the older literature indicates loss of coherency while more recent literature provides evidence of pseudomorphic island growth. This ambiguity may result from the fact that in the more recent literature the Au (111) surface was in its reconstructed *23 x √3* herringbone state while, while in the older literature the gold surface was likely bulk-terminated. The one-dimensional relaxation associated with the reconstruction represents a surface compression of about 4%. Thus, the Cu wetting layer may be pseudomorphic on the reconstructed Au (111) surface while maintaining only partial coherency on the bulk-terminated surface.

We report on results for stress evolution in this system in both vacuum and electrolyte for the first Cu wetting layer. In various electrolytes we observed that at the completion of the coherent wetting layer the change in surface stress was -0.65 Jm^{-2}. Stress evolution in vacuum showed complex behavior in that the stress change achieved a maximum of + 0.26 Jm^{-2} at ~ 0.5 ML and decayed to a value of + 0.07 Jm^{-2} at full monolayer coverage. In the vacuum experiments RHEED data indicated that the Au (111) surface was bulk-terminated. Total energy calculations were made within the local-density approximation for a pseudomorphic Cu ML on bulk-terminated Au (111) which yielded a surface stress change of + 1.6 Jm^{-2}. Embedded Atom Method potentials were fit to values of surface stress and surface energy for Cu (111) and Au (111) derived from the first principles results, and these potentials were employed in molecular dynamic simulations that were performed in order to sort out the details of stress evolution.

Analysis of the simulation results together with experiment have allowed us to develop an understanding of the stress evolution during the growth of the Cu wetting layer on bulk-terminated Au (111). The only model consistent with our results is based on a mechanism of dislocation generation in the wetting layer involving second layer island formation on the as yet uncompleted first ML and interlayer adatom transport resulting in the nucleation of dislocations in the wetting layer. This type of dislocation nucleation mechanism was apparently first suggested by Bauer[1], van der Merwe[2], and more recently by Comsa[3] and Hwang[4]. Our understanding of the vacuum result suggests that anion adsorption plays and important role during stress evolution of this system in electrolytes.

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