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Formation and Vibrational Entropy-Driven Disordering of Mo(100) and W(100) Surface Alloys M.S. ALTMAN, K.L. MAN, Y.J. FENG, C.T. CHAN, Hong Kong University of Science and Technology — Atoms that are deposited on a surface of a dissimilar material may either remain on the surface or they may become incorporated in a surface or bulk alloy. Although the energetic differences between alloy and overlayer structures at T = 0 can now be understood from first principles in many systems, the entropic contribution to the system free energy, which governs the equilibrium structure, is less well understood. The formation and stability of Cu, Ag and Au-induced c(2x2) alloys at the Mo(100) and W(100) surfaces have been investigated with low energy electron microscopy and diffraction. The dependence of the c(2x2) diffraction intensity upon metal deposition flux reveals that alloy formation is governed by atomistic processes that are analogous to those that dictate overlayer island nucleation. An order-disorder transition is also observed that converts the surface from ordered alloy to disordered overlayer structure. Combined with knowledge of energetics that is obtained from first principles calculations, a comparison of disordering temperatures for alloys of the different metal species and substrates provides information on the decisive contribution of vibrational entropy to the system free energy. Effective Debye temperatures for metal adatoms are determined that are substantially lower than bulk values, but exhibit the expected mass and bond strength dependence.Vibrational entropy may also play a role in the stability of alloys at other surfaces.

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