[S-18]

Ordered Mn surface alloys on Au(001)

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The atomic structures of two different, ordered Mn surface alloys on Au(001) were studied by the low energy electron diffraction (LEED) I/V (spot intensity versus incident electron energy) analysis. The first one was formed of a subsurface c(2x2) alloy layer beneath 1 monolayer (ML) thick Au capping layer, 1ML Au/1ML c(2x2) Au-Mn/Au(001). The atomic structure was just like the bulk terminated Au3Mn(001) with negligible surface relaxation. The second alloy film has a tri-layer structure on Au(001), c(2x2) 1ML Au-Mn/1ML Mn/1ML c(2x2)Au-Mn/Au(001). Contrary to the first one, we found large contraction of the layer spacing in the alloy and strong buckling of Mn in the surface layer. We discussed the energetics relevant to the formation of the observed alloy structures.