Epitaxial fcc Fe Films on Cu(100)

A recent Letter by Pescia *et al.*[1] reports controversial magnetic properties for thin films of fcc Fe epitaxially grown on Cu(100). Our studies reveal that Fe on Cu(100) does not, as claimed, grow in a layer-by-layer manner, and structural imperfections are the likely source of the controversy. Indeed, from elementary thermodynamics layer-by-layer growth is not expected for high surface-free-energy metals (e.g., V, Fe, or Co) on low surface-free-energy substrates (e.g., Cu or Ag) when the interfacial bonding is relatively weak (as it is between noble and transition metals).[2]

Auger-amplitude plots can, as Pescia *et al.* claim, indicate layer-by-layer growth if a series of straight line segments is clearly and decisively a better fit to the data points than a smooth curve. Whenever such plots are published, readers are advised to sketch in a smooth curve and judge for themselves. A smooth curve is expected if either agglomeration or interdiffusion is important.

Our results are based on an extensive, multitechnique study; however, the data of Fig. 1 are sufficient to rule out a layer-by-layer growth mode since at a coverage of 1 monolayer (ML), Fe on Cu(100) exhibits a strong forward-scattered peak at 45° (this peak even appears at 0.1 ML Fe). This peak should not be present if the Fe were a flat, uniform monolayer on the Cu(100) surface, as is 1-ML Cu on Ni(100).[3] Instead, on the order of half the Fe atoms must have either Cu or Fe atoms in the next layer above [as in the 2-ML Cu on Ni(100) case]. Therefore, either the 1-ML Fe on Cu(100) actually forms Fe double layers covering half the Cu(100) surface, or Cu atoms segregate out onto the Fe layer, or a combination of both. Our other data indicate that both processes occur.[4] We find that at or slightly above 300 K, the segregating Cu and the partially exposed Cu(100) substrate gradually get buried in the range of 1-3 ML Fe, so that the films of Pescia *et al.* were strongly agglomerated and somewhat intermixed with Cu.

Our results show that the Fe agglomeration and the Cu segregation may be avoided by depositing at a substrate temperature of 100 K to suppress the surface diffusion that mediates these effects. For 3-ML Fe, subsequent annealing to 345 K to achieve a smooth and well-ordered film is possible (only at higher temperatures do Fe agglomeration and Cu segregation then begin). Such films exhibit much improved magnetic properties, being ferromagnetic at 300 K with a strong perpendicular anisotropy.[5] However, for 1- and 2-ML Fe films the agglomeration begins upon annealing to $\sim$200 and $\sim$250 K, respectively, and if the films are inadequately annealed they contain many irregularities such as steps, islands, or adatoms.

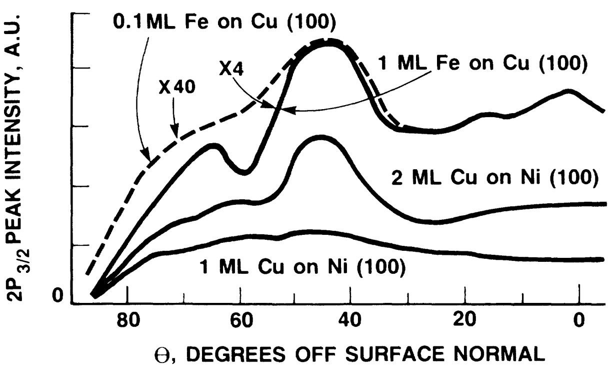

FIG. 1. The angle-resolved XPS intensity ($\langle 100\rangle$ azimuth) of the $2p_{3/2}$ peak of the deposited element. The strong forward-scattered feature at 45° demonstrates that 0.1 and 1 ML Fe deposited at 300 K on Cu(100) do not lie flat on the surface, as does 1 ML Cu on Ni(100).

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