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## Intermixing at Cr<sub>n</sub>/Cu(001) interface and the magnetic properties of Cr

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We study the effects of interfacial intermixing on electronic structure and magnetic properties of thin Cr<sub>n</sub>/Cu film ( $n=1$  or  $3$ ) by using the method of ab initio full potential linear muffin-tin orbital (FP-LMTO). The formation of Cr-Cu in the subsurface layer is energetically favorable. The antiferromagnetic ordering of in-plane in Cr/Cu is found to be energetically favorable more than that of out-plane. In order to simulate the interfacial intermixing in Cr/Cu, we use the system of 50:50 CrCu alloy layer on the surface or at the interface, as well as the sandwich of Cr/(Cr<sub>x</sub>Cu<sub>1-x</sub>)<sub>n</sub>/Cu (where  $x = 0.25, 0.50,$  and  $0.75$  for  $n=1, 2,$  and  $3,$  respectively). The Cr sites in 50:50 CrCu alloy layers on Cu(001) are very high spin-state, and antiferromagnetically aligned in the plane (or out-plane) of the film. Our result for the energetics of surface alloying shows clearly that the Cr magnetization is rather intricate, depending on the degree of interface mixing and the change of interlayer distance at the Cr/Cu interface.