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Chromium surfaces and Cr monolayers atop Fe have greatly enhanced magnetizations relative to bulk. The Cr (100) surface is ferromagnetic with a spin polarization of 3.00; the (110) surface is antiferromagnetic. A Cr monolayer is ferromagnetic atop either the (100) or (110) Fe surfaces; the former has a large polarization of 3.63.
In transition metals the itinerant nature of the d electrons makes magnetism sensitive to the local environment. Consequently the presence of a dissimilar neighbor, as found in an interface, or the absence of some neighbors, as found at a surface, may cause considerable changes in the local magnetic properties. Bulk chromium has an antiferromagnetic (AF) ground state modulated by an incommensurable spin-density wave (SDW). The SDW is in one of the <100> directions with a wavelength of approximately 2\( \times \)1 lattice spacings (1). The magnetization at the maximum is \(0.59 \mu_B\) (2). It is found that the addition of small amounts of impurities produces a simple AF structure (3) with a magnetic moment of approximately \(0.67 \mu_B\). This structure demands that <100> planes contain atoms of only one spin direction. Consequently the (100) surface is expected to possess ferromagnetic order. Evidence of this planar ferromagnetism is found in electron-capture spectroscopy (4) and in angle-resolved photoemission experiments (5-7).

The (100) surface of Cr has been examined theoretically (8-11): the ferromagnetic surface is found to have a large magnetic moment between 2.5 and 3.0 \(\mu_B\) and a high surface Curie temperature.

The <110> planes cut the simple AF bcc lattice so that an equal number of up and down spins are
encountered. The (110) surface should therefore be AF. There have been two photoemission experiments on the Cr (110) surface (12,13). Here we present results of calculations for the magnetic and electronic properties of the (100) and (110) surfaces of Cr, and for the systems consisting of a monolayer of Cr deposited on the Fe (100) and (110) surfaces. We use a Slater-Koster parametrized tight-binding scheme in which the one- and two-center integrals are fitted to the bulk band structure. The single-site electron-electron interaction is treated self-consistently in a Hartree-Fock approximation. This scheme has been previously used and has produced excellent agreement with both experimental data and state-of-the-art calculations (10).

**THE CHROMIUM (100) SURFACE**

We obtain a surface spin polarization of 3.00, an enhancement by a 5.1 factor from the bulk SDW maximum, and much larger than the corresponding enhancements in Fe and Ni (14,15). The enhancement can be attributed to the large number of unpolarized d holes in the bulk and to the decreased bandwidth at the surface, which leads to a stronger effective magnetic interaction. Elements like Fe or Ni, with fewer available
unpolarized holes, experience smaller changes in the same local environment. Most d-holes occur in the minority subband, which is essentially concentrated in a single peak structure entirely above the Fermi level. The spin polarization of the second layer is opposite to that of the surface layer, in agreement with the AF of chromium. Its spin polarization is (-1.56). Those of the third through sixth layers are 1.00, (-0.93), 0.86, and (-0.85) respectively. A similar deep penetration of the enhanced surface magnetization was found in the Fe (100) surface (14), although there the effect is much smaller. Each Cr atom feels the larger exchange splitting of its neighbor towards the surface and responds by increasing its own; this is, in the case of Cr, an energetically very inexpensive process.

THE CHROMIUM (110) SURFACE

We obtain, as the ground-state configuration, a two-atom unit surface cell with AF ordering. The surface spin polarization is 2.31. This value is smaller than that for the (100) surface as one would expect, since the (110) surface atom has six nearest neighbors, as opposed to four in the (100) surface. We were unable to find a ferromagnetic locally stable minimum.
The spin polarization in the second layer agrees in direction with the perfect AF structure but its spin polarization of 1.00 is considerably smaller than that of a second-layer (100) atom, 1.56.

CHROMIUM MONOLAYERS ON IRON

We have calculated the spin polarization of a Cr monolayer atop the Fe (100) surface to be 3.63, with a ferromagnetic arrangement pointing oppositely to the underlying Fe substrate. This value is the largest spin polarization we have ever calculated, or found in the literature, for a transition-metal system.

Insight into this result may be gained by comparing it with the dilute FeCr alloy. Neutron scattering (16) results show that the isolated Cr atom spins point oppositely to the surrounding Fe bulk and have a polarization of 1.2 electrons. This latter result presumably stems from the stronger electron-electron interaction in Fe, and a stronger exchange splitting which helps Cr increase its own splitting and magnetization.

The combined effect of diminished number of neighbors and stronger exchange results in the calculated large Cr moment. We may understand the AF coupling by noting that Mn, an antiferromagnet,
is the element intermediate between Fe and Cr.

Figure 1 shows the DOS projected on the Cr monolayer and on the underlying Fe layer. The most obvious feature is the enormous minority DOS at the Cr monolayer. It is a consequence not only of the surface band narrowing, but also of the absence of Fe majority holes to which the Cr minority holes (same spin) may be coupled. These two facts leave a subband with essentially no effective nearest neighbors, and therefore very narrow.

We find, for the (110) configuration, that the ground state consists of a ferromagnetic Cr monolayer with its spins oriented in the direction opposite to the Fe substrate, similar to the Cr on Fe (100) arrangement. The spin polarization of the Cr is 2.25 electrons, smaller than the pure Cr surface.

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FIGURE

Fig. 1: The d-orbital component of the projected density of states. (a) The chromium (100) monolayer. (b) The iron (100) interface layer. Solid lines are states with the spin orientation of the minority bulk iron states; dashed lines correspond to the majority states.
Figure 1

Density of states (atom)$^{-1}$(Ry)$^{-1}$

Energy (Ry)
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