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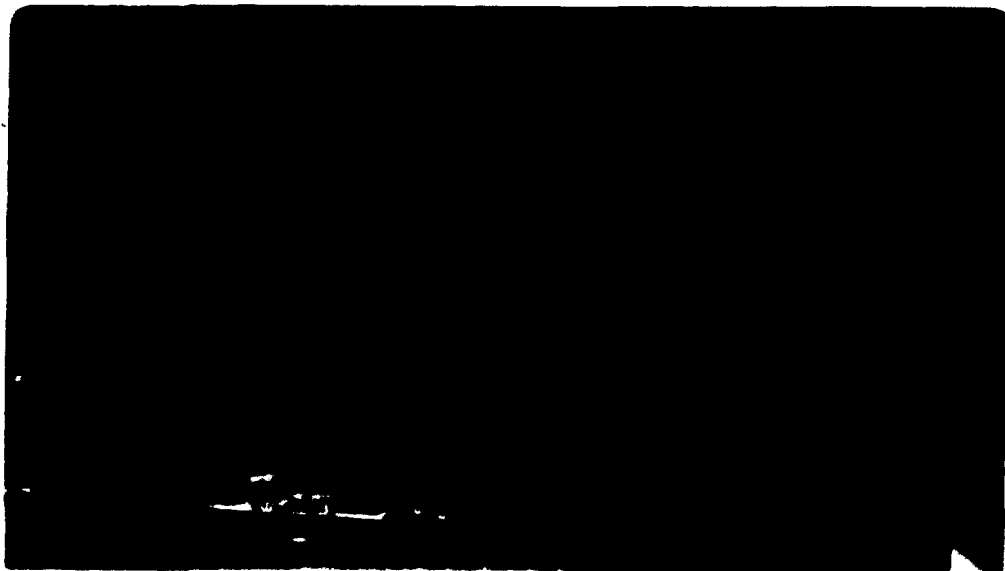
Materials & Molecular Research Division

ELECTRONIC AND MAGNETIC STRUCTURE OF CHROMIUM
SURFACES AND CHROMIUM MONOLAYERS ON IRON

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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.

Surface Magnetism
Chromium Surfaces
Chromium Overlayers on Iron

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DISCLAIMER

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 21 lattice spacings (1). The
magnetization at the maximum is 0.59 μ_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 μ_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 μ_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 $\underline{d}$-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 2.3↑. 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.

ACKNOWLEDGMENTS

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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
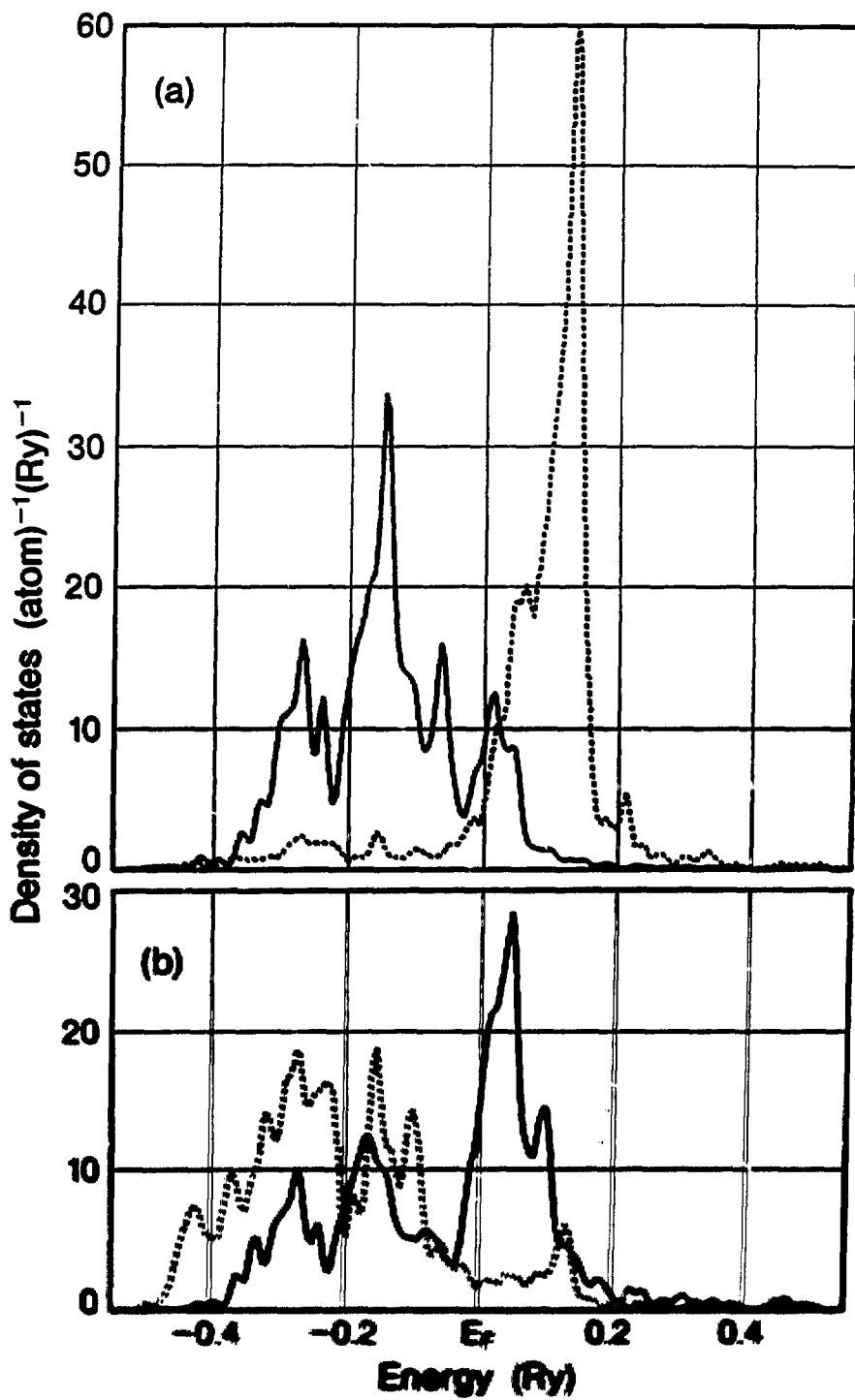correspond to the majority states.

Figure 11

Figure 11