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Computer-Based Microscopic Description of the Structure and Properties of Materials

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Preface

This volume contains the papers that were presented at the 1985 MRS Fall Meeting in Symposium R, entitled "Computer-based Microscopic Description of the Structure and Properties of Materials." The purpose of the symposium was to bring together the various communities that use computers to predict, describe, or simulate the atomic and electronic structure and properties of materials. It was the first such symposium at an MRS meeting. It brought together those whose main focus is the electronic structure and those whose main focus is the dynamics of atomic motion.

Electronic structure approaches, based on the quantum mechanical wave equation (Hartree-Fock, density functional theory, pseudopotentials, band-structure theory, molecular-orbital theory, etc.) have been quite successful in obtaining very accurate descriptions of the electronic properties of given atomic arrangements, but have been limited in searching for stable atomic configurations or doing dynamics at finite temperatures. On the other hand, "molecular dynamics" approaches have traditionally absorbed all electronic structure information into phenomenological interatomic potentials, which makes dynamical calculations at finite temperatures feasible and efficient. These two communities have been evolving separately, but, in the last few years, there have been tendencies to borrow from each other or merge the two approaches. The symposium was meant to foster this interchange of ideas, and to bring these two main communities together with others, including those who design and use special-purpose computers, those who simulate experimental data, and other related fields.

The symposium was sponsored by the NSF (Steven R. Williams), the ARO (John C. Hurt), NASA (Joseph R. Stephens), Oak Ridge National Laboratory (through Energy Conversion and Utilization Technologies; Joseph A. Carpenter, Jr.) and AFOSR (John E. Lintner). We are thankful for their generous support.

Last of all, we would like to thank Joan Pidot, Kitty Boccio, Barbara Cardella, Lorraine Miro and Janet Hutsko for their professional and supportive secretarial services.

Jeremy Broughton
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STRUCTURAL, ELECTRONIC, AND MAGNETIC PROPERTIES OF SURFACES, INTERFACES, AND SUPERLATTICES*

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ABSTRACT

Advances in all-electron local density functional theory approaches to complex materials structure and properties made possible by the implementation of new computational/theoretical algorithms on supercomputers are exemplified in our full potential linearized augmented plane wave (FLAPW) method. In this total energy self-consistent approach, high numerical stability and precision (to 10^{-4} in the total energy) have been demonstrated in a study of the relaxation and reconstruction of transition metal surfaces. Here we demonstrate the predictive power of this method for describing the structural, magnetic and electronic properties of several systems (surfaces, overlayers, sandwiches, and superlattices).

I. INTRODUCTION

Recent progress in the fabrication and property modifications of artificial materials, such as thin films, sandwiches, and modulated structures, have generated a great deal of interest. The excitement surrounding this development lies in the possible discovery and synthesis of new materials with desired properties to specification, and permitting new phenomena to be investigated and novel devices to be made. Concurrently, advances in computational/theoretical approaches have developed capabilities of yielding precise results and making successful predictions possible. In coordination with experimental studies, these theoretical efforts serve to advance the appearance of new and quite unexpected phenomena and to promote their understanding.

In this paper, we study theoretically the structural and magnetic properties of (1) 3d transition metal surfaces and (2) 3d transition metals as overlayers or sandwiches and superlattices with noble metals. For the surfaces and sandwiches, we solve the local spin density functional equations[1] self-consistently using the full-potential linearized augmented plane wave[2] (FLAPW) method; and the linear muffin-tin orbital[3] (LMTO) method is employed for CrAu(001) superlattice with various thicknesses.

II. TRANSITION METAL SURFACES

We start with the discussion of surface magnetism of 3d transition metals. Since the surface atoms have lower coordination and reduced symmetry, it is now widely recognized that there is an enhancement of the magnetism near the surface layer as a result of localized surface states[4]. In Table I we summarize the calculated results of the magnetic moment for surface atoms and, for the sake of comparison, their bulk counterparts.

For ferromagnetic Fe and Ni (100) and (110) surfaces, the magnetic moments are enhanced by about 10 ~ 30% from their bulk values. It is not surprising that the (100) surface has the largest enhancement simply

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because the surface atom has the lowest coordination numbers.

A more dramatic case is Cr(100), which undergoes a surface ferromagnetic phase transition with a largely enhanced moment of $2.49\mu_B$. Recently, this has been confirmed by angle-resolved photoemission experiments[5]. By contrast to the results obtained for Cr(001), using a spin-polarized total energy approach and a study of the multilayer relaxation of V(100), we predict a stable paramagnetic state for this surface. Further, for the paramagnetic V(001), we obtain a 9% contraction of the topmost interlayer spacing accompanied by an expansion of the second interlayer spacing by 1%, which is in excellent agreement with LEED[6]. Analysis of the electronic structure of V(100) shows that the surface states which are characteristic of the occurrence of surface magnetism in bcc Cr and Fe is located about 0.3 eV above E_F. A comparison between Cr and V also serves to illustrate the role played by these surface states in the enhancement of the surface magnetism in the case of Cr(001).

Table I. Calculated magnetic moments (in μ_B) for 3d transition metals

		V	Cr	Fe	Ni
surface	(100)	0	2.49	2.98	0.68
	(110)			2.63	0.63
bulk		0	0.59	2.15	0.56

III. METALLIC OVERLAYERS AND BIMETALLIC SANDWICHES

Having illustrated the effect of surface states on the magnetic and electronic properties of transition metal surfaces, our next goal was to explore the possibility of inducing 2D magnetism in a controlled way. It turns out that the transition metal and noble metal interfaces are of special interest[7,8] because: (1) a close to perfect epitaxial growth due to a nearly perfect match of the 2D lattice translational vectors for (001) Cr (or Fe) and Au (or Ag) (the (100) plane of the transition metal layers are rotated by 45 with respect to that of the noble metal, and the stacking has atoms in the four-fold hollow site of adjacent atomic planes); and (2) the dissimilarity of the electronic structures between transition metals and noble metals which ensures minimum hybridization between localized surface (interface) states near E_F and the underlying non-magnetic noble metal d-band.

In order to understand the electronic and magnetic structures at the interface, we first examined the crystal structure. This was carried out using a total energy approach for both Au/Cr/Au(001) sandwiches and AuCr coherent modulated structures. We find that the interaction between noble and transition metals is local in nature; this manifests itself in an

Au-Cr interlayer spacing which is an average of the bulk fcc Au and bcc Cr spacings; the bulk Cr and Au structures are essentially unperturbed away from the interface.

Selected results for the magnetic moments calculated within each atomic sphere at the Au/Cr interface are presented in Table II. As an aid in understanding the underlying physics and to emphasize its 2D nature, we focus first on results for the experimentally unattainable free monolayer Cr(001) film. A large magnetic moment of $4.12\mu_B$ is obtained which is close to the atomic limit and substantially larger than that of bulk antiferromagnetic Cr metal ($0.59\mu_b$). Surprisingly, when a monolayer of Cr(001) is deposited onto Au(001), the magnetic moment of the Cr overlayer decreases by only a small amount from the free monolayer value to $3.70\mu_B$. This extremely large moment - the largest value reported for a transition metal other than for Mn - is 50% greater than that of the surface layer in Cr(001) predicted theoretical ($2.49\mu_B$) or derived experimentally ($2.4\mu_B$). Also surprising is the finding that this substantially enhanced moment is only moderately reduced (to $3.10\mu_B$) when the Cr overlayer is itself covered by a Au layer. Apparently, the hybridization between Au and Cr is far less than expected. A very similar result was obtained, $2.95\mu_B$ per Cr atom, when the (1x1) Cr/Au coherent modulated structure was studied with the linear muffin-tin orbital approach (Table II) to be discussed later. Since Cr is a notorious getter, the retention of this enhanced 2D magnetization in either the single sandwich or superlattice structures might make its observation much easier.

Similar investigations have also been performed for monolayers of Fe and V adsorbed on Ag(001). For Fe-Ag there is a close matching of the lattice constants but a 5% mismatch for V-Ag or -Au. As in the case of Cr/Au(001), large magnetic moments, $2.96\mu_B$ (Fe) and $2.0\mu_B$ (V), are found for the adsorbate monolayers. The magnetic moment of the Fe overlayer on Ag(001) is remarkably close to the theoretical magnetic moment of the surface layer of an Fe(001) film ($2.98\mu_B$) - again indicating a lack of interaction with the substrate. The result for V/Ag(001) is much more surprising since, like the bulk, the surface layer of V(001) is not magnetic. We thus have the remarkable prediction that an overlayer of V on Ag(001) is magnetically ordered with a sizable magnetic moment ($1.98\mu_B$) which is almost as large as the moment of Fe in bulk Fe. (If confirmed, this will be the first solid material for which elemental vanadium demonstrates magnetic ordering.) The origin of magnetic ordering is not negative pressure since, in fact, the matching to the Ag(001) substrate results from a reduced lattice constant for V by 5%. For both the Fe and V overlayers we find - despite some hybridization between the d bands of the adsorbate and substrate - that the adsorbate-localized surface state bands retain their quasi-2D behavior for these systems. This behavior is further demonstrated for a monolayer of Fe sandwiched by Ag(001). The magnetic moment of Fe is only slightly decreased from that of the overlayer of Fe/Ag(001) to $2.80\mu_B$. [Similarly, a moment of $2.92\mu_B$ on the Fe site is found for an Au/Fe/Au(001) sandwich.] However, when a monolayer of V(001) is sandwiched by Ag(001), the vanadium layer becomes paramagnetic.

The sensitivity of the magnetic ordering of V to its metallic environment is further illustrated by calculations with two layers of V on Ag(001): In this case the interface layer atoms remain essentially in the paramagnetic state and the surface layer has a moment of $1.15\mu_B$ which is substantially reduced from that of the single-overlayer value ($1.98\mu_B$). We thus have the result that a Ag substrate is more amenable for the magnetism of a V monolayer than is another V layer.

IV. COHERENT MODULATED STRUCTURES (SUPERLATTICES)

In order to examine the magnetic coupling between Cr layers in the multilayer structure, thickness effects have been examined by varying the Cr and Au layer numbers in the CrAu(001) coherent modulated structure.

We start with the simplest case - a CrAu [1*1] superlattice (hereafter we specify a system by a notation [n*m], where n and m denote the number of Cr and Au layers). A non-spin polarized calculation shows a very high density of states at E_F associated with Cr d states, and a Stoner instability to a ferromagnetically ordered state since the calculated Stoner factor $N(E_F)I_{xc} = 1.34$. In a spin polarized calculation, a sizable magnetic moment ($2.94\mu_B$) is actually found on the Cr atoms while a small moment ($0.10\mu_B$) is ferromagnetically induced on the Au atoms. This value of the magnetic moment is very close to that obtained ($3.1\mu_B$) for a monolayer of Cr sandwiched by Au (cf. Table II).

Table II. Theoretical layer by layer magnetic moments (in μ_B) for specified cases (with estimated uncertainties of $\pm 0.03\mu_B$). S and (S-n) indicate surface and subsurface layers. The last column shows the spin-polarized energy (in eV). CMS, coherent modulated structure.

	Cr	Nearest Au	*E*(para.) − *E*(spin-pol.)
Cr monolayer	4.12	. . .	1.69
1 Cr/Au(001) overlayer	3.70	0.14	0.78
2 Cr/Au(001)	2.90 (*S*), −2.30 (*S* − 1)	−0.08	0.60
Au/Cr/Au(001) sandwich	3.10	0.14 (*S*), 0.13(*S* − 2)	0.38
(1×1) Au/Cr CMS	2.95	0.10	0.25
	Fe	Nearest Cu, Ag, Au	
Fe monolayer	3.20	. . .	1.34
1 Fe/Cu(001)	2.85	0.04	0.70
1 Fe/Ag(001)	2.96	0	1.14
2 Fe/Ag(001)	2.94 (*S*), 2.63 (*S* − 1)	0.05	1.15
Ag/Fe/Ag	2.80	0	0.88
Au/Fe/Au	2.92	0.08	0.97
	V	Nearest Ag,Au	
1 V/Au(001)	1.75	0.04	0.10
1 V/Ag(001)	1.98	0.06	0.14
2 V/Ag(001)	1.15 (*S*), < 0.05 (*S* − 1)	0	0.08
Ag/V/Ag	0	0	. . .
Cr/Fe/Au(001)	3.10 (Cr), −1.96 (Fe)	−0.04 (Au)	0.68
Fe/Cr/Ag(001)	2.30 (Fe), −2.40 (Cr)	−0.09 (Ag)	0.52

For superlattices with thicker constituent layers, a reduction of the magnetic moment at the interface may be expected due to greater hybridization. The calculated magnetic moments for some CrAu(001)

Table III. Magnetic moments (in μ_B) within atomic spheres for CrAu (001) superlattices with various thicknesses. Each layer is specified by atomic type, Cr or Au, ordering assumed (F=ferro and AF=antiferromagnetic) and interplanar distance from the interface layer (i).

superlattice type	layer	magnetic moments
[1*1]F	Cr_i	2.94
	Au_i	0.10
[1*1]AF	Cr_i	3.00
	Au_i	0.00
	Cr_i	-3.00
	Au_i	0.00
[1*3]	Cr_i	3.01
	Au_i	0.07
	Au_{i-1}	0.04
[3*3]	Cr_{i-1}	-1.07
	Cr_i	1.89
	Au_i	0.09
	Au_{i-1}	0.01
[5*5]	Cr_{i-2}	0.68
	Cr_{i-1}	-0.79
	Cr_i	1.65
	Au_i	0.08
	Au_{i-1}	0.00
	Au_{i-2}	0.01

superlattices with various thicknesses is listed in Table III. Interestingly, in the case of CrAu [1*3], the magnetic moment on Cr is not reduced but even slightly enhanced by an additional Au layer. The interface Au d band becomes wider than that of the Au monolayer but not enough to overlap with the Cr d band region; the Cr d band is essentially

the same as that of CrAu [1*1]. We may conclude that the Cr monolayer sandwiched by Au has a sizable magnetic moment ($3\mu_B$) independent of Au thickness.

For sandwiches with thicker Cr, the magnetic moment of the interface Cr is substantially reduced from that of the monolayer Cr with Au but still much larger ($1.89\mu_B$ and $1.65\mu_B$ in CrAu [3*3] and [5*5], respectively) than that of bulk Cr ($0.59\mu_B$). The large reduction of the interface moment is due to broadening of the interface Cr d band caused by hybridization with inner Cr d states. We can expect such a large moment on the interface Cr atoms ($1.5\mu_B$) even for thicker sandwiches than five layers of Cr, because the innermost Cr atoms in CrAu [5*5] already have a magnetic moment very close to the bulk value.

Finally, we discuss the effect of magnetic interactions between the layers. As shown in Table III, interplanar magnetic interactions between the Cr layers always result in antiferromagnetic couplings, while those between the interface Cr and Au layers result in ferromagnetic ones. In order to study the interplanar magnetic interaction in more detail, we compare the total energies for CrAu [1*1] superlattice where the ferromagnetic Cr(001) monolayers are coupled ferromagnetically ([1*1]F) or antiferromagnetically (in which case the unit cell is doubled, [1*1]AF) along the [001] direction. We found that the antiferromagnetic coupling is preferred by 11 mRy/formula unit. This difference will, of course, vary with Au thickness and reach a point - with perhaps 3-5 Au layers separating the Cr monolayers - where the interaction becomes so weak that a reasonable external magnetic field would align the monolayers ferromagnetically. The magnetic moment of the interface Cr in [1*1]AF is slightly larger than that in [1*1]F (see Table III). This enhancement of the moment and also the similar enhancement in [1*3] mentioned above can be understood by the fact that the antiferromagnetic coupling between the ferromagnetic Cr(001) monolayers works destructively on the magnitude of the moments under the ferromagnetic constraint along the [001] direction.

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