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Magnetism in surfaces: an orbital-resolved study

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Abstract

In this paper we carry out a detailed orbital (ℓ–m–m_s) resolved study of the way in which the local magnetic moment changes as we go from the bulk to a planar or a rough surface. For a rough surfaces (FCC Ni (1 0 0) and BCC Fe (1 0 0) surfaces) we shall concentrate on specific structures on them and study the way in which local environment affects the local magnetic moment. Results will be shown for Fe, Co and Ni planar surfaces.
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1. Introduction

The enhancement of magnetic moment at the surfaces of transition metals is a well established fact [1–4]. Development in experimental techniques along with extremely accurate first-principles, self-consistent local spin-density (LSDA) based calculations have only strengthened this belief. This enhancement is attributed to the reduced symmetry and coordination number at surfaces. This in turn results in band narrowing and hence enhancement of the paramagnetic density of state at E_F [5]. Stoner-like arguments then lead to an enhancement of the local magnetic moment. The purpose of this paper is to carry out a detailed orbital resolved study of surface magnetic moments on both planar and rough surfaces.

Though it is in general true that band narrowing leads to enhancement of the surface magnetization, when we scanned the individual orbital components, we found not all of them contribute to this enhancement. In fact few of the orbital (ℓ–m) resolved components were actually magnetically suppressed. In discussing surface enhancement the role of d-band is often emphasized. We found that the s and p bands also play a significant

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role, specially in Ni (1 0 0) and hexagonal closed packed (HCP) Co (1 0 0) surfaces, where the enhancement is feeble. The moment enhancement is largest in Fe BCC (1 0 0), where the majority band (in bulk) is not saturated and less in Ni and Co where the majority band is almost saturated. Eriksson et al. [6] and Alden et al. [5] suggest that, less saturated the majority band in bulk more the possibility of enhancement at the surface. For Ni thin films, almost the whole of the enhancement at the surface was due to the $d_{x^2-y^2}$ orbital, but for this state the majority band was more saturated than the three t_{2g} states in the bulk. It is therefore of importance that we carry out a detailed orbital decomposed study of magnetism at a surface before we can make statements with confidence.

There have been numerous theoretical studies of thin films and surfaces, both for free standing thin films, as well as for those on substrates, using different methods. The theoretical approaches have been carried out in essentially three different approaches:

(i) Single slab geometry with boundary matching Green functions [2,8–11].
(ii) Slabs in a three-dimensional supercell, well separated by *empty space* with charge but no atoms [13–18]. The assumption is that the slabs separated by sufficiently wide empty spaces do not interact with one another.
(iii) A Green function technique making use of the two-dimensional periodicity on flat surfaces and treating the direction perpendicular to the surface by a real-space method. This was implemented within the tight-binding linearized muffin-tin orbitals method (TB-LMTO) by Skriver and Rosengaard [19] and used to study Ni surfaces by Alden et al. [5].

By construction, the first and last of these approaches takes proper account of broken symmetry at the surface. The second approach introduces artificial periodicity. However, it is believed that it does render accurate results when carried out to convergence [7].

Haydock et al. [20] proposed a technique for the calculation of projected and integrated density of states which was based entirely on *real space* representations and therefore did not necessarily make any use of translational symmetry of any kind. This *recursion method* also yielded the energy moments of the projected density of states and most related physical quantities with *controlled accuracy*. Extensive work has been carried out to identify the errors in the recursive procedure and both analytical and numerical estimates of errors are available [21–24]. With this method it is possible to control errors. Earlier, we have applied this method to study the Ni thin films [25]. One of the overriding advantage of the recursion method above others is the possibility of studying rough surfaces.

In this communication we extend our scheme of combining the recursion method with the TB-LMTO to study unsupported (1 0 0) thin films of transition metal elements Ni (FCC), Fe (BCC) (both planar and rough) and Co (FCC), Co (HCP) (only planar). They are surrounded by layers of *empty spheres* carrying the charge spilled out of the slabs. We have obtained the layer resolved local density of states and the local magnetic moment for these thin films. Our main interest was to see, how individual orbitals contributed to surface magnetism and how the bulk degeneracies are lifted for the surface states. All our thin films were nine layers thick surrounded by layers of empty spheres to mimic the spilled out charge. We had earlier seen that for a nine layer thick slab, the central layer local density of states is almost indistinguishable from the bulk.

2. Methodology and results

The recursion method can be combined with any electronic structure basis which yields a sparse representation of the Hamiltonian. The TB-LMTO based on the work by Andersen and co-workers [28] is ideal in this respect as it yields both a *minimal* basis set and an almost nearest-neighbour tight-binding like Hamiltonian.

The second order TB-LMTO Hamiltonian is written in terms of potential parameters and the

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