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LAYER PROJECTED MAGNETIC MOMENTS OF ATOMS OF A ROUGH SURFACE

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Abstract

We use a pair of coupled continuum equations to generate a rough surface which models molecular beam epitaxy. Using these equations, we generate a rough Fe surface on Ag substrate. We then use the Recursion method coupled with the tight binding linear muffin tin orbital method (TB-LMTO) for the density of states and magnetic moments of different atoms having curvature on the rough surface. We also calculate the magnetic moments of atoms of different layers below the surface atoms. We observe that the magnetic moments of atoms on the rough surface varies with the local curvature but for the atoms of sub-surface layers, the dependence is not prominent.

1 Introduction

Magnetic and non-magnetic overlayers prepared by various vapour deposition techniques on substrates invariably lead to the formation of rough surfaces. Considerable work has gone into the description and quantification of surface roughness [1]. Experimentally one can access such descriptions, for example, through glancing angle X-ray scattering experiments [2, 3, 4, 5, 6, 7]. We observed earlier that [8] the local magnetic moment in a solid is strongly influenced by the immediate environment, so it varies randomly across the rough surface. Atomic binding energy of systems occur due to the collective behaviour of interacting itinerant electrons. The study of the effect of extended defects, like surfaces and interfaces on itinerant electron binding energy, takes us a step further. The surface co-ordination number of an atom differs quite a bit as compared to that of the bulk solids [9]. When a surface is formed, the environment of the atoms at the surface is different from the bulk. Atoms at the surface have fewer neighbours as compared to the bulk and consequently their bonding to the solid is weaker.

We shall generate a rough surface and then obtain the local density of states at various positions on the surface using a local spin density approximation based on the electronic structure technique. The exact method for generating the rough surface is not important to our results, except for the fact that it will fix the degree of roughness of the resulting profile. We have chosen the coupled stochastic equations model suggested by [10] and in a modified form by [11], since we have some understanding of the roughness produced in [10]. Moreover, the model has, we believe, built in it many of the physical mechanisms involved in the deposition process. These include:

(i) a randomly fluctuating incoming flux,

(ii) a shape rearrangement to minimize the chemical potential which leads to a surface diffusive current proportional to the gradient of the local chemical potential and

(iii) an evaporation-accretion process arising out of finite substrate temperatures.

Our proposal for the study of surface magnetization roughness will not change qualitatively if we use any other model for generating the rough surface. For the electronic structure technique we have used the tight-binding linearized muffin-tin orbitals method proposed by Andersen [12, 13] coupled with the recursion method of [14, 15].

Both these methods have been described in great detail in the referenced papers. We shall indicate here the main results we have used for our analysis. The "second order" Hamiltonian generated self-consistently within the TB-LMTO has the form,

$$\mathbf{H}^{(\sigma,i)} \;=\; \mathbf{E}_{\nu}^{(\sigma,i)} + \mathbf{h}^{(\sigma,i)} - \mathbf{h}^{(\sigma,i)}\;\mathbf{o}^{(\sigma,i)}\;\mathbf{h}^{(\sigma,i)} \tag{1}$$

where,

$$\mathbf{h}^{(\sigma,i)} = \sum_{RL} \left(C_{RL}^{(\sigma,i)} - E_{\nu,L}^{(\sigma,i)} \right) \quad \mathbf{P}_{RL} + \sum_{RL} \sum_{R'L'} \Delta_{RL}^{1/2(\sigma,i)} \; S_{RL,R'L'}^{(i)} \; \Delta_{R'L'}^{1/2(\sigma,i)} \quad \mathbf{T}_{RL\alpha,R'L'\alpha'}$$

- R labels the position of a given atom and i indicates which layer below the surface R sits. $L = \ell, m$ are composite angular momentum indices, σ is the spin index (either $\uparrow$ or $\downarrow$).
- $C_{RL}^{(\sigma,i)}, o_{RL}^{(\sigma,i)}$ and $\Delta_{RL}^{1/2(\sigma,i)}$ are the potential parameters of the TB-LMTO method.
- $S_{RL,R'L'}^{(i)}$ is the short-ranged screened structure matrix, which depends only on the geometry of the underlying lattice. This may be different at the surface because of surface dilatation.
- $\mathbf{P}_{RL}$ and $\mathbf{T}_{R'L'}$ are the projection and transfer operators in Hilbert space $\mathcal{H}$ spanned by tight-binding basis $\{| \, RL\rangle\}$

Using this Hamiltonian, the recursion method provides the Green functions:

$$\begin{aligned} G_{RL,RL}^{(\sigma,i)}(E) &= \langle R, L| \left(E\mathbf{I} - \mathbf{H}^{(\sigma,i)} \right)^{-1} |R, L\rangle \\ &= \cfrac{1}{E - \alpha_1 - \cfrac{\beta_1^2}{E - \alpha_2 - \cfrac{\beta_2^2}{\ddots \quad \cfrac{\beta_{N-1}^2}{E - \alpha_N - T(E)}}}} \end{aligned} \tag{2}$$

$T(E)$ is the appropriate *terminator* obtained from the initial part of the continued fraction. The terminator preserves the herglotz analytic properties of the approximated Green function. The imaginary part of the Green function gives us density of states.

The spheridized local charge density within an atomic sphere centered at $\mathbf{R}$ can be obtained from

$$\rho_(\sigma)^{(i)}(r_R) = \frac{1}{4\pi} \sum_l \left[m_{Rl}^{(0)} \phi_{l\sigma} + 2m_{Rl}^{(1)} \phi_{l\sigma} \dot{\phi} r_R + m_{Rl}^{(2)} \left(\dot{\phi}_{\sigma l}(r_R)^2 + \phi_{\sigma l}(r_R) \ddot{\phi}_{\sigma l}(r_R) \right) \right]$$

where the energy moments are

$$m_{Rl}^{(n)} = -\frac{1}{\pi} Im \int_{-\inf}^{E_F} dE G_{RL,RL}^{(\sigma,i)}(E)(E - E_{\nu,Rl})^n \tag{3}$$

The $\phi_{\sigma l}(r_R)$ are the radial solutions of the Kohn-Sham equations within the atomic sphere centered at R. The local Hartree and Exchange-correlation potentials are functionals of the local

charge densities. For the expression for the exchange correlation we have used the Barth-Hedin functional [16]. The magnetization density within that sphere is:

$$M^{(i)}(r_R) = \rho_{\uparrow}^{(i)}(r_R) - \rho_{\downarrow}^{(i)}(r_R) \tag{4}$$

The charge and magnetization densities are then input into the self-consistency iterations using the LSDA. The total energy includes contributions up to dipoles from the charge layer in the empty spheres at the surface. After convergence, the magnetic moment in the atomic sphere centered at R in the i-th layer from the surface is calculated from:

$$M^{(i)}(r_R) = \int_0^{s_R} M^{(i)}(r_R) r_R^2 dr_R \tag{5}$$

2 The input parameters

The potential parameters used in equation (1) are layer dependent and different from those of the bulk. To get the starting potential parameters we did a number of super-cell calculations. We used a unit cell of tetragonal structure of 12-30 atomic spheres. The empty spheres containing the charge but no atoms take care of the charge leakage. We take a unit cell by varying the number of layers for Fe and empty spheres. Using these parameters we did a recursion calculation and observed that density of states obtained in different layers of (100) plane match very well with the result obtained from the LMTO(in Fig. 1).

3 Rough surface formation

We should reiterate at the outset that the procedure for the generation of a rough surface profile is immaterial to the analysis of local magnetic moment distribution on a rough surface. However, for the analysis of the nature of roughness in the moment distribution and its correlation with the roughness in the profile requires us to choose a particular generation procedure. We shall choose here the coupled stochastic equations similar to those proposed by Sanyal *et al* [10], modified later by [11]. The coupled equations have been discussed quite extensively in the referenced articles and the reader is referred to them for details.

Figure 2 displays the rough surface produced using the coupled equations. We should note that, on the rough surface, translational symmetry is lost both perpendicular and along the surface. The roughness of such surfaces has been traditionally measured by the scaling exponent α of the height-height two-point correlation function

$$\begin{aligned} S(\underline{r} - \underline{r}', t - t') &= \ll h(\underline{r}, t) h(\underline{r}', t') \gg - \ll h(\underline{r}, t) \gg \ll h(\underline{r}', t') \gg \\ &\simeq |\underline{r} - \underline{r}'|^{2\alpha} \quad \text{for the saturated surface } |t - t'| > t_c \end{aligned}$$

The height-height correlation function for the rough surface is presented in Fig. 3.

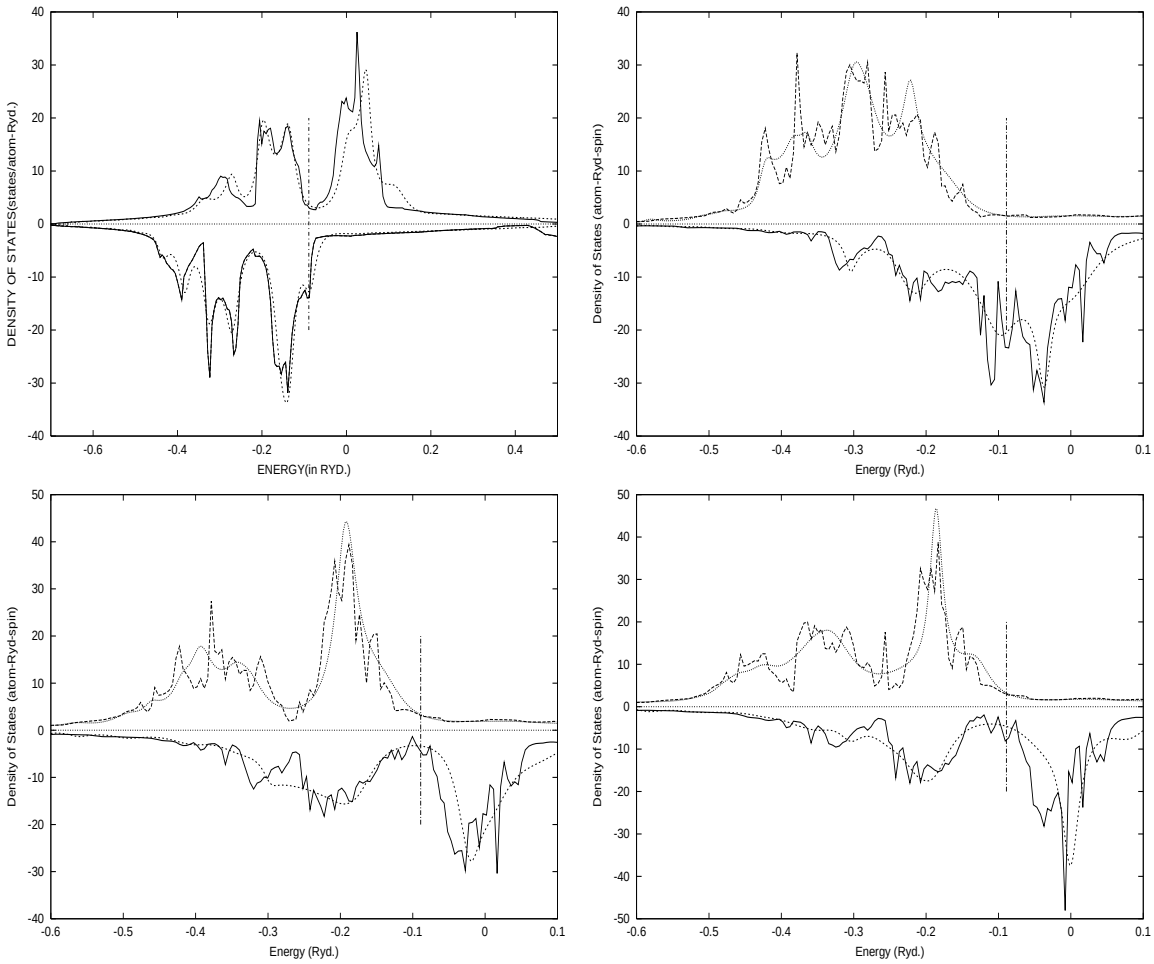

Figure 1: The layer resolved density of states of a bulk Fe [*top left*], surface layer[*top right*], sub-surface S-1 [*bottom left*] and sub-surface S-2 [*bottom right*] on a [100] plane. Both the K-space and recursion method are used. The vertical line shows the bulk Fe Fermi energy

4 Computation details and results

We have used a real space cluster of 6402-11011 atoms (depending on the position of the starting site on the surface of 50 X 50 atoms) which remains within the 16th shell from the starting site. We generated 30 pairs of recursion coefficients accurately. We performed our calculation in around 50 points of different parts of the roughsurface having different curvature and as well as the subsurface atoms to determine the density of states and magnetic moments. The density of state of bulk Fe and some points on the rough surface is presented in Fig 4.

The average magnetic moment of atoms of different curvature is given in Table 1 . In all calculations, we observe an oscillatory convergence of magnetic moments from the surface to the bulk value.

The average magnetic moment at the negative curvature is larger, as expected, but it is observed that in the sub-surface layer the domination of curvature on magnetic moment is not

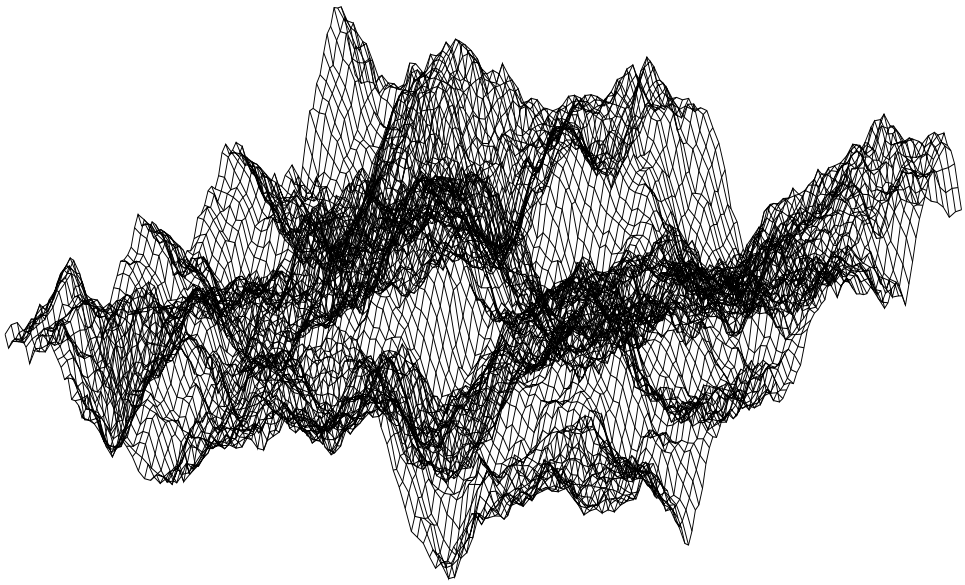

Figure 2: A part of the rough surface produced using coupled equations of [11].

Curvature	Layer				
	S	S-1	S-2	S-3	S-10
-4	3.13	2.23	2.40	2.29	2.26
-2	3.05	2.22	2.39	2.28	2.26
0	2.99	2.18	2.39	2.28	2.26
2	2.97	2.21	2.38	2.28	2.26
4	2.89	2.21	2.38	2.28	2.26

Table 1: The layer projected average magnetic moment of atoms on different surface points and subsurface points of a rough surface.

prominent.

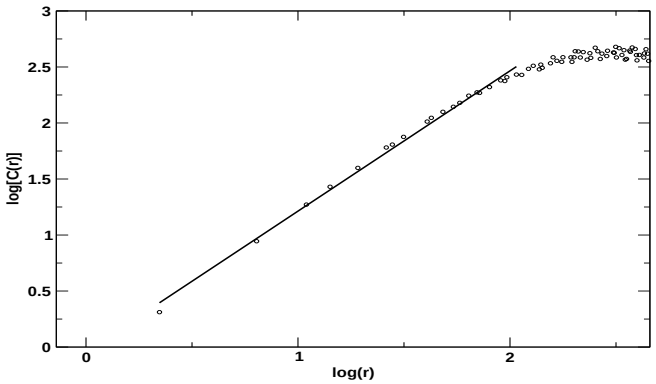

Figure 3: Height-height correlation function C(r) plotted against r. Using the equation $C(r) = \langle (h_i - \langle h \rangle)^2 \rangle^{1/2}$. As C(r) $\sim r^{\alpha}$, we obtain a roughness exponent, $\alpha = 0.68$.

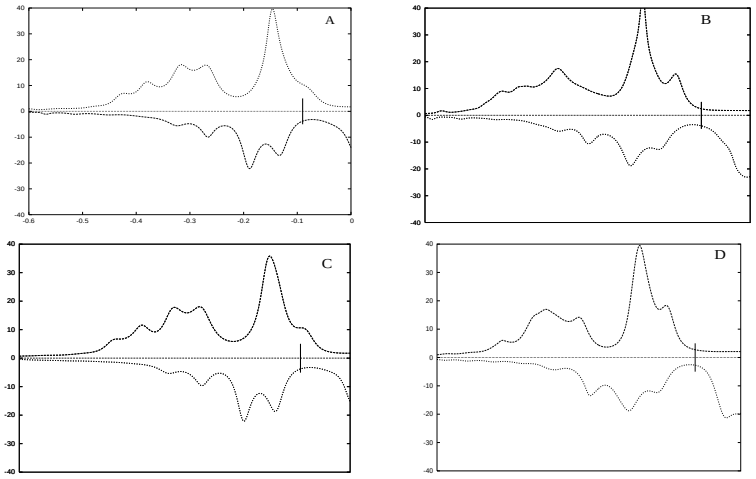

Figure 4: Density of states of Bulk Fe (A) and some other points with different curvature (B-D)

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References

[1] Barabasi A L and Stanley H E, *Fractal concepts in surfa ce growth* (Cambridge University Press) (1995).

[2] Kundu S, Hazra S, Sanyal M K, Mandal S K, Chaudhuri S and Pal A K, *J. Phys. D: Appl. Phys.*, **31**, L 73, (1998).

[3] Sanyal M K, *Radiat. Phys. Chem.*,**51**, 487, (1998).

[4] Sanyal M K, Datta A, Banerjee S, Srivastave A K, Arora B M, Kanakaraju S and Mohan S, *J. Sync. Rad.*, **4**, 185,(1997).

[5] Sinha S K, Feng Y P, Melendres C A, Lee D D, Russell T P, Satija S K , Sirota E B and Sanyal M K, *Physica*, **A231**, 99, (1996).

[6] Sanyal M K, *Current Science*,**60**, 880, (1994).

[7] Sinha S K, Sanyal M K, Satija S K, Majkrzak C F, Neumann D A, Homma H, Szpals S, Gibaud A and Markoc H, *Physica B*,**198**, 72, (1994).

[8] Huda A.-U. and Mookerjee A., *Jour. of Mag. and Mag. Mater.*, **267**, 97 (2003).

[9] Fu C L, Freeman A J and Oguchi T, *Phys. Rev. Lett.* **54** 2700 (1985)

[10] Sanyal B, Mehta A and Mookerjee A, *J. Phys.: Condens. Matter* **11** 4367 (1999)

[11] Huda A -U, Dutta O and Mookerjee A, *Int. J. Mod. Phys.* **B 17(6)**, 2981 (2003)

[12] Andersen O. K., *Phys. Rev. B***12** 3060 (1975).

[13] Andersen O. K. and Jepson O. *Phys. Rev. Lett.* 53, 2571 (1984).

[14] Haydock R, Heine V and Kelly M J, J. Phys. C Solid State Phys. **5** 2845 (1972)

[15] Haydock R, Heine V and Kelly M J, Surf. Sci. **38** 139 (1973)

[16] Barth U V and Hedin L, *J. Phys. C: Solid State Phys.* **5**, 1692 (1972).