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Variation of Binding Energy of Atom on 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 use Recursion method coupled with TBLMTO method for the density of states of different point on the rough surface. Then we use Burke orbital peeling method for the binding energy of Fe atoms on the different points of rough surface.

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 observe earlier that [9] the local magnetic moment in a solid is strongly influenced by the immediate environment, so it vary 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 a atom differs quite a bit as compared with 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 electronic structure technique and hence the binding energy using Burke orbital peeling method [10]. The exact method for generating the rough surface is not material 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 suggestedby [11] and in a modified form by [12], since we have some understandingof the roughness produced [11]. 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 [13,14]coupled with the recursion method of [15,16].

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,

$$H^{(\sigma,i)} = E_{\nu}^{(\sigma,i)} + h^{(\sigma,i)} - h^{(\sigma,i)} o^{(\sigma,i)} h^{(\sigma,i)}$$

Where

$$h^{(\sigma,i)} = \sum_{R} (C_{RL}^{(\sigma,i)} - E_{\nu L}^{(\sigma,i)}) P_{RL} + \sum_{RL} \sum_{R'L'} \Delta_{RL}^{1/2(\sigma,i)} S_{RLR'L'}^{i} \Delta_{R'L'}^{1/2(\sigma,i)} T_{RL,R'L'}$$

- R labels the position of a given atom and i indicates which layer below the surface R sites. L =l,m are composite angular momentum indeces, σ is the spin index (either ↑ or ↓).
- C, o, Δ are the potential parameters of the TB-LMTO method.
- $S_{RLR'L'}$ 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.
- P_{RL} and $T_{RLR'L'}$ are the projection and transfer operators in Hilbert space H spanned by tight-binding basis {|RL>}

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

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$$G^{(\sigma,i)}_{RL.RL}(E) = \left\langle R,L \left| \left(EI - H^{(\sigma,i)}\right)^{-1} \right| R,L \right\rangle$$

$$= \cfrac{1}{E-\alpha_1 - \cfrac{\beta_1^2}{E-\alpha_2 - \cfrac{\beta_2^2}{\ddots \\ \cfrac{\beta_n^2}{E-\alpha_N - T(E)}}}}$$

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.

1.1 Orbital peeling method [10]

If we have two systems one consists of an adatom and the surface and the second system is the surface without the adatom. If the hamiltonian for the first system is H_0 and the second is H_1. The density of states of two systems are respectively,

$$N_0 = -\frac{1}{\pi}\,\mathrm{Im}\,Tr\left[E + i\delta - H_0\right]$$

$$N_1 = -\frac{1}{\pi}\,\mathrm{Im}\,Tr\left[E + i\delta - H_1\right]$$

where the limit as δ tends to zero is implied.

The structural energy of these systems are,

$$U_0 = \int_{-\infty}^{E_F} EN_0(E)dE$$

$$U_1 = \int_{-\infty}^{E_F} EN_1(E)dE$$

The interaction energy is given by,

$$W = U_1 - U_0$$

$$= \int_{-\infty}^{E_F} (E - E_F)\Delta N dE$$

where $\Delta N = N_1 - N_0$. Using the matrix identity

$$Tr(EI - H)^{-1} = \frac{\partial}{\partial t}\log\det(EI - H)$$

We obtain,

$$\Delta N = \frac{\partial}{\partial E}\log\frac{\det(EI - H_1)}{\det\left(EI - H_0\right)}$$

Now the first (α-1) rows and columns of the matrix [E-$H_{1,0}$] are deleted to get the peeled green function and after a little bit of mathematics, we find the energy difference

$$W = 2\left[\sum_i z_i + \sum_i p_i + (N_p - N_z)E_F\right]$$

where N_p and N_Z are the number of poles and zeroes respectively.

II. 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 super-cell calculations.We used a unit cell of tetragonalstructure 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 this parameters we did a recursion calculation and we observe that density of states obtained in different layers of (100) plane match very well with the result obtained from the LMTO (in Fig. 1).

III. 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 which is such that we have knowledge about the nature of its resulting surface profile. We shall choose here the coupled stochastic equations similar to those proposed by Sanyal [11], modified later by [12]. The coupled equations have been discussed quite extensively in the referenced articles and the reader is referred to them for details.

Figure. 4 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 have been traditionally measured by the scaling exponent α of the height-height two-point correlation function

$$S(r-r',t-t') = \left\langle\left\langle h(r,t)\,h(r',t')\right\rangle\right\rangle - \left\langle\left\langle h(r,t)\right\rangle\right\rangle\left\langle\left\langle h(r',t')\right\rangle\right\rangle$$

$$= |r-r'|^{2\alpha} \quad \text{for the saturated surface } |t-t'| > t_c$$

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

IV. 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 remain within the 16th shell from the starting site. We generated 30 pairs of recursion coefficients accurately. We perform our calculation in around 350 points on the rough surface to determine the energy required to knock off an atom from the surface. We have also calculated the curvature of that corresponding points. The result of our calculation is given in the fig. 5. We observe that the energy required to knock off an atom is higher in positive curvature or groove than that of negative curvature or mounds. This was exactly what we mentioned in coupled continuum equation.

Fig. 5 and the negative slope of the regression line clearly show that the binding energy is higher in the area of positive curvature or in the groove and it is lower in the area of negative curvature or mounds. It is expected because the surface atom at the mound has less coordination number than that of the groove.

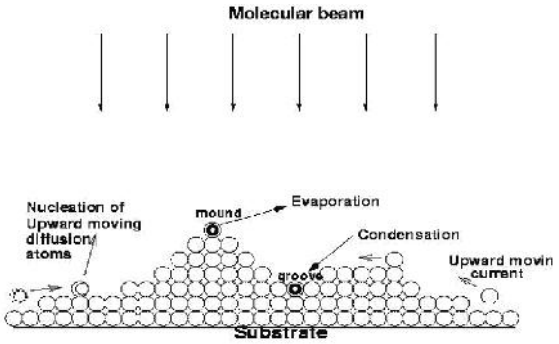

Fig. 1. A Pictorial Description of the model.

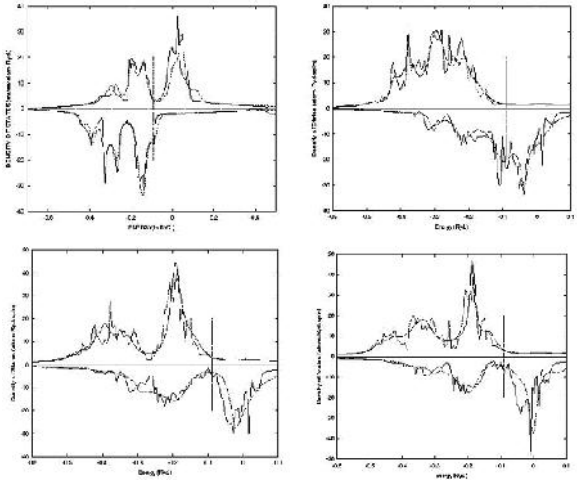

Fig. 2. The layer resolved density of states of a bulk Fe [top-left, surface layer [top-right], sub-surface S-1 [bottom-left] and sub-surface S-2 [bottom-right] on a [100] plane. Both the K-space and recursion method is used. The vertical line shows the bulk Fe Fermi energy

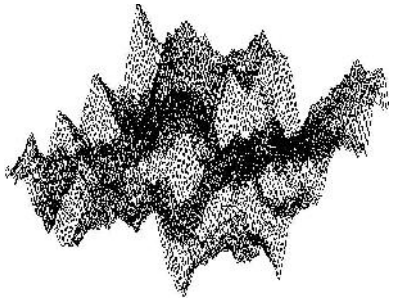

Fig. 3. A part of the rough surface produced using coupled equations of [20].

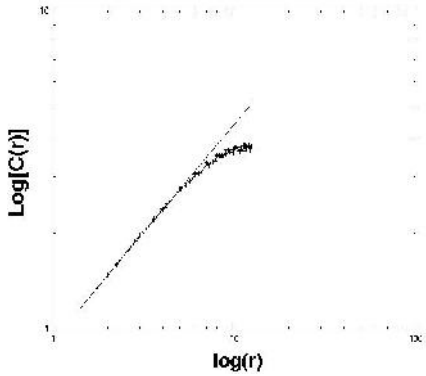

Fig. 4. Height-height correlation function C(r) plotted against r. Using the equation $C(r) = \left\langle \left(h_i - \langle h \rangle\right)^2 \right\rangle^{1/2}$. As $C(r) \sqcup r^{\alpha}$, we obtain α=0.68.

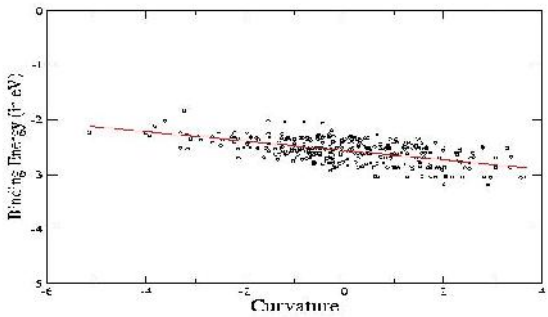

Fig. 5. The energy required to Knock off atoms-curvature scatter diagram and its regression curve. The regression line is E=2.5623+ 0.086331 C.

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1. Barabasi A L and H E Stanley, 1995, Fractal concepts in surface growth, Cambridge University Press.
2. Kundu S, S. Hazra, M K Sanyal, S K Mandal, S Chaudhuri and A K Pal , *J. Phys. D: Appl. Phys.*, 31, L 73 (1998).
3. Sanyal M K , 1998, *Radiat. Phys. Chem.*, 51, 487, Sanyal M K, Datta A, Banerjee S, Srivastave A K, Arora B M, Kanakaraju S and Mohan S, *J. Sync. Rad.*, 4, 185 ,(1997).
4. Sinha S K, Y P Feng, C A Melendres, D D Lee, T P Russell, S K Satija, Sirota E Band Sanyal M K, 1996 *Physica*, A231, 99.
5. Sanyal M K, 1994, *Current Science*, **60**, 880.
6. Sinha S K, M K Sanyal, S K Satija, C F Majkrzak, D A Neumann, H Homma, S Szpals, A Gibaud and H Markoc, 1994 *Physica* B, **198**, 72.
7. Huda A.-U. and A Mookerjee, 2003, *Jour. of Mag. and Mag. Mater*., **267**, 97.
8. Fu C L, A J Freeman and T Oguchi, 1985, *Physical Review Letter* **54,** 2700.
9. Burke N. R., 1976, *Surf. Sci.* **58,** 349.
10. Sanyal B, A Mehta and A Mookerjee, *Int.1999, Jour. Mod. Phys.* **B 11,** 4367.
11. Huda A -U, O Dutta and A Mookerjee, *Int. 2003, Jour. Mod. Phys.* **B 17(6)**, 2981.
12. Andersen O. K. , 1975, *Phys. Rev.* B, 12, 3060.
13. Andersen O. K. and O Jepson, 1984, *Phys. Rev. Lett,* **53**, 2571.
14. Haydock R, V Heine and M J Kelly, 1972, *Jour. Phys. C : Solid State Phys.* **5,** 2845.
15. Haydock R, V Heine and M J Kelly, *Surf. Sci.* **38,** 139 (1973).