

THE $t_{2g} - e_g$ BAND SPLITTING OF ATOMS ON A ROUGH SURFACE

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ABSTRACT

Any deposition techniques lead to the production of rough surfaces. Some researchers proposed a pair of coupled continuum equations, which models the molecular beam epitaxy. This model was used to generate a rough surface of Fe, which is deposited on a Ag substrate. Then use of recursion method of Haydock with the parameter of tight binding linearized muffin tin orbital method of Anderson revealed that the t_{2g} and e_g bands are nondegenerate at bulk and [100] plane but near the rough surface, the degeneracy is broken and splitting of density of states depends on the curvature of the surface.

Key words: Rough surface, Band splitting, Atoms, Recursion model

INTRODUCTION

During the last few decades, the thin film deposition techniques have become an emerging area of research for its technological importance. The resulting films may be as thin as a few atomic layers or as thick as several micrometers. The deposition of a thin film is a critical step in the manufacture of integrated technology over the last 50 years. The thin films are widely used in recording devices. Other applications requiring thin films include solar cells, mechanical coatings, and more recently, microelectronic systems and micro-fluid devices.

There are several methods that physicists use to grow thin films. Some of the famous methods include pulse laser deposition (PLD), chemical vapor deposition (CVD) and molecular beam epitaxy (MBE). Most of the useful devices made of thin films need smooth interfaces for good contact. However, roughening is also an inevitable part of surface formation. Magnetic and non-magnetic over-layers prepared by various vapor deposition techniques on substrates invariably lead to the formation of rough surfaces, so that understanding the basic mechanism leading to surface roughness is important. This understanding may then be used to grow film in regimes where roughening is reduced or absent. The dynamics of surface growth by atomic deposition have been the focus of interest over recent years (Bak *et al.* 1987, Jaeger and Nagel 1992, Jaeger *et al.* 1996,

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Mehta and Barker 1994a, Mehta and Barker 1994b, Mehta *et al.* 1996a, Mehta *et al.* 1996b, Das and Kotlyar 1994, Huda *et al.* 2003). Several theoretical attempts (Barabasi and Stanley 1995) at the understanding of kinetic roughening have been made, through discrete and continuum models, which are motivated by experiments.

Considerable work has gone into the description and quantification of surface roughness. Experimentally, one can access such descriptions, for example, through grazing-angle X-ray scattering experiments (Kundu *et al.* 1998, Sanyal 1994, 1998, Sanyal *et al.* 1997, Sinha *et al.* 1996). It was observed that (Huda and Mookerjee 2003) the magnetic moment in a solid is a local property, so it varies randomly across the rough surface. The density of states of a system as well as many electronic properties depends on the collective behavior of interacting itinerant electrons.

The study of the effect of extended defects like surfaces and interfaces on itinerant electron the study of d-bands electrons takes us a step further. The surface coordination number of an atom differs quite a bit compared to that of the bulk solids (Fu *et al.* 1985). When a surface is formed, the environment of the atoms at the surface is different from the bulk. Atoms at the surface have fewer neighbors compared to the bulk, and consequently their bonding to the solid is weaker.

In this work, the splitting of d-bands was studied near the surface.

METHODOLOGY

In order to study the d-band splitting near the rough surface, we require a rough surface in our study. δ There are many models of molecular beam epitaxy. In this work we used the model proposed by (Huda *et al.* 2004), where the coupled continuum equations are given by,

$$\frac{\partial h(\bar{r}, t)}{\partial t} = D_h \nabla^4 h(\bar{r}, t) - \tau + \eta_h(\bar{r}, t) \quad (1a)$$

$$\frac{\partial \rho(\bar{r}, t)}{\partial t} = D_\rho \nabla^2 \rho(\bar{r}, t) + \tau \quad (1b)$$

where the transfer term is given by:

$$\tau = v |\nabla^2 h(\bar{r}, t)| [1 - \Theta(\nabla^2 h(\bar{r}, t))] - \mu \rho(\bar{r}, t) |\nabla^2 h(\bar{r}, t)| \Theta(\nabla^2 h(\bar{r}, t)) \quad (1c)$$

where, $\theta(x)$ is 1 for $x > 0$ and 0 otherwise.

The above equations are used to produce a rough surface as shown in Fig. 1

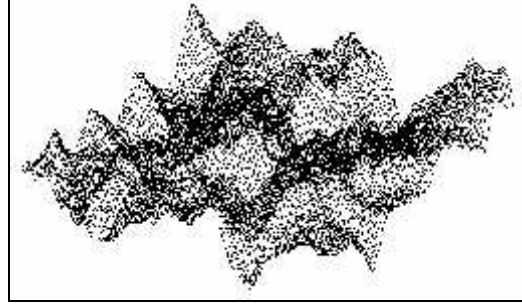


Fig. 1. A part of rough surface produced using coupled continuum equations.

The second order Hamiltonian generated self-consistently within the TB-LMTO [20] has the form

$$H^{(\sigma,i)} = E\gamma^{(\sigma,i)} + h^{(\sigma,i)}O^{(\sigma,i)}h^{(\sigma,i)} \quad (2)$$

where,

$$h^{(\sigma,i)} = \sum_{RL} \left(C_{RL}^{(\sigma,i)} - E\gamma_L^{(\sigma,i)} \right) P_{RL} + \sum_{RL} \sum_{RL'} \Delta_{RL}^{\frac{1}{2}(\sigma,i)} S_{RL,R'L'}^{(i)} \Delta_{RL}^{\frac{1}{2}(\sigma,i)} T_{RL\alpha R'L'\alpha'}$$

- Here R labels the position of a given atom and I indicates which layer below the surface R sits, $L = 1, m$ are composite angular momentum indices, σ is the spin index (either \uparrow or \downarrow).
- $C_{RL}^{(\uparrow,i)}$, $O_{RL}^{(\uparrow,i)}$ and $\Delta_{RL}^{\frac{1}{2}(\sigma,i)}$ 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 underlying lattice. We observed that it is different at different position of rough surface because of surface dilation.
- P_{RL} and $T_{RL,R'L'}$ are the projection and transfer operators in Hilbert space \mathbf{H} spanned by tight binding basis $\{|RL\rangle\}$.

The Green's function is defined as,

$$G_{ii}(z) = G_{RL,RL}^{(\sigma,i)} = \langle R, L | (EI - H^{(\sigma,i)})^{-1} | R, L \rangle$$

$$= \frac{1}{E - \Gamma_0 - \frac{S_1^2}{E - \Gamma_1 - \frac{S_2^2}{E - \Gamma_2 - \frac{S_2^2}{\vdots}}}}}$$

$$E - \Gamma_n - \frac{S_n^2}{T_n(z)}$$

$T_n(z)$ 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 charge and magnetization densities are then input into the self-consistency iterations using the LSDA.

The input parameters used in equation (2) 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 Fe and empty spheres. Using the parameters we did a recursion calculation and observe that the density of (100) plane match well with the result obtained from the LMTO.

RESULTS AND DISCUSSION

Both the recursion method and TB-LMTO method were used to calculate the density of states of bulk Fe. In Fig. 2, the d-bands spin resolved density of states of bulk Fe is presented. It is observed that the three t_{2g} and two e_g bands are degenerated in case of bulk Fe.

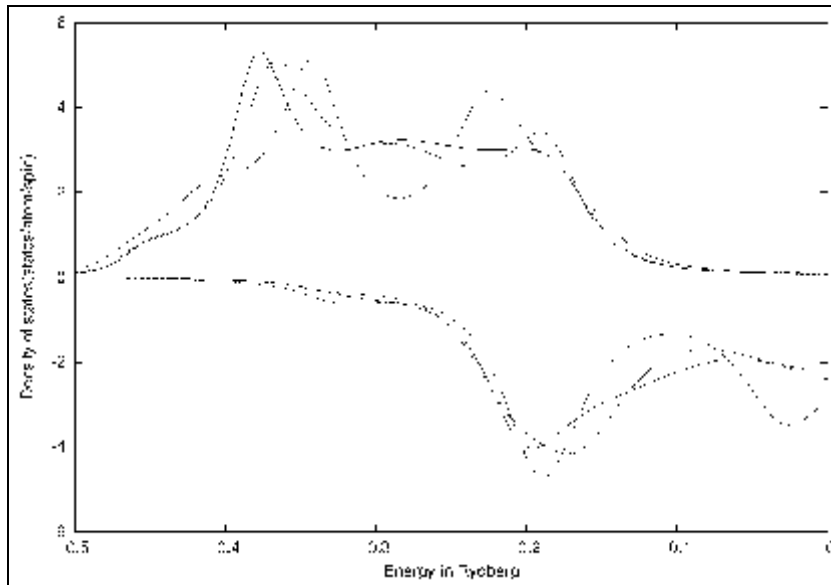


Fig. 2. Spin projected density of states of t_{2g} band of Fe on the rough surface. There are clearly three separate t_{2g} bands.

Then by using the recursion method of Haydock *et al.* (1972) for obtaining the density of states of atoms on the [100] plane. In order to obtain the potential parameters of the surface, a supercell calculation was done of 12 - 20 atoms. The potential parameters of these layers are later used in recursion method to obtain the density of

states of recursion method. In present calculation, it was observed that there was no splitting in t_{2g} and e_g bands of Fe. The authors also observe that in case of atoms of an [100] Fe plane, there was splitting in t_{2g} and e_g .

The recursion method of Haydock (1972) was used for obtaining the density of states of atoms on the rough surface. It was known that the recursion method is the best one to calculate the density of states where the periodic symmetry is broken, i.e., at the surfaces, interfaces etc. For this purpose, a real space cluster of 6402 - 11011 atoms (depending on the position of the starting site of the rough surface of 50×50 atoms) was used, which remain within the 16th shell from the starting site. The starting parameters of the rough surface are obtained from the linearized muffin tin orbital method. To obtain the potential parameters of the surface a supercell calculation was done of 12 - 20 atoms. The potential parameters of these layers are later used in recursion method to obtain the density of states of recursion method.

The layer dependent potential parameters, obtained from [100] Fe plane are then used as the starting parameter of the rough surface calculation. The self consistently iteration was done in such a way, that the total energy and charges of consecutive two calculations remain within 0.00001 limit.

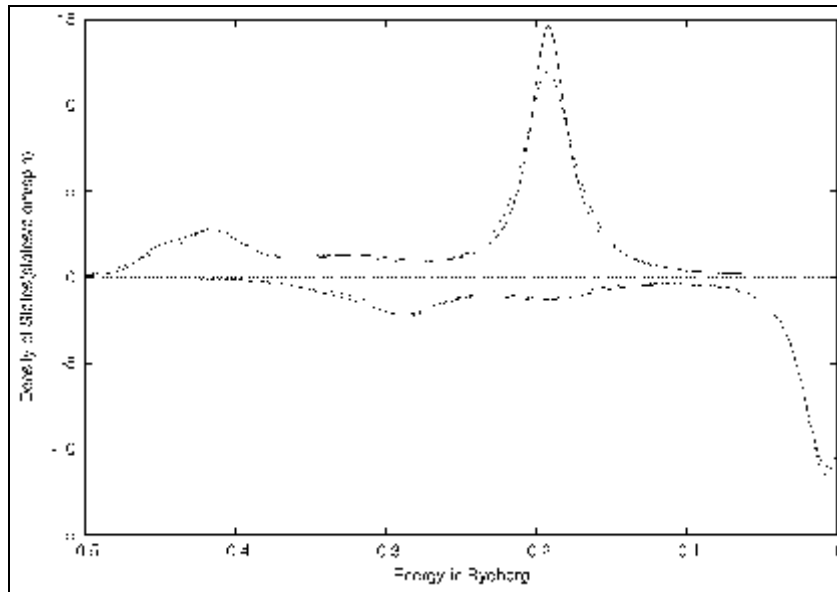


Fig. 3. Spin projected density of states of e_g band of Fe on the rough subsurface layer S-1. There are clearly two separate e_g bands.

Fig. 2 represents the spin-projected density of states of t_{2g} bands Fe atom on a specific point of rough surface. In this case unlike the bulk atom or [100] plane atom, the degeneracy of t_{2g} bands are broken. The degeneracy of e_g bands is broken here also.

The density of states of sub-surface layers were calculated as well. Fig. 3 represents the e_g band of surface layer S-1. The authors also calculated t_{2g} and e_g bands of different subsurface layers and it was found that the splitting of d bands decreased as it went deeper in the bulk.

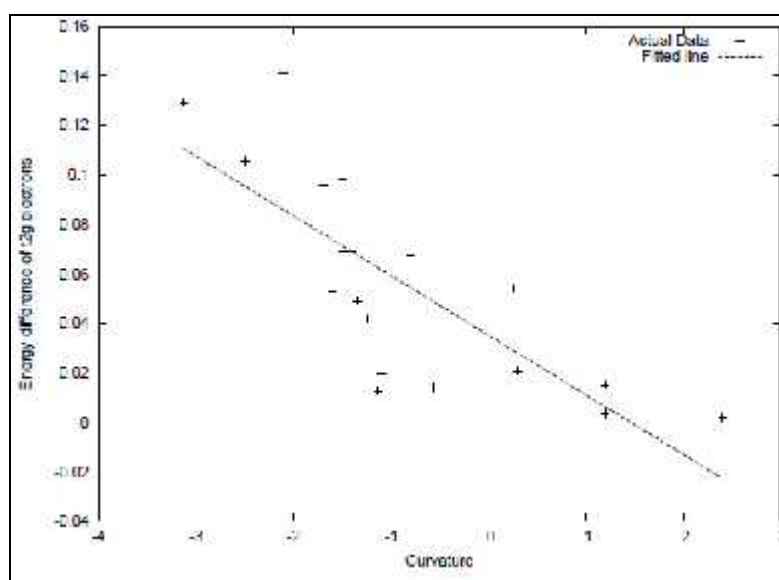


Fig. 4. A plot of energy difference of t_{2g} electrons at various points of curvature on the rough surface.

The energy difference between the t_{2g} and e_g electrons was calculated at different points of the rough surface. It was observed that the energy differences between the t_{2g} electrons are higher than the e_g electrons. Fig. 4 represents the energy differences of t_{2g} electrons at the various points of rough surface having different curvature. From Fig. 4, it is clear that at negative curvature points i.e. at the points of mounds, the energy differences are higher and at the point of positive curvature, the energy differences are lower. The negative slope curve suggests that the splitting of electron energy depends on the type of curvature of the surface.

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(Received revised manuscript on 14 November, 2014)