Superficies y Vacío 1, 174-178(1989)

LOCAL DENSITY OF STATES OF A V-Ta INTERFACE. IS IT MAGNETIC?

R. de Coss, A. Noguera and R. Baquero

Departamento de Física del Instituto de Ciencias
Universidad Autónoma de Puebla
Apdo. Postal J48 Puebla, Pue. 72570, México

We have used the bulk orthogonal d-tight-binding parameters for V and Ta from the work of Harrison and we have used the Green's function matching method as cast by García-Moliner and Velasco to calculate the Local Density of States for the V-Ta interface. This method takes in principle full account of the interface perturbation and therefore allows the use of the bulk tight-binding parameters. We found that the V side interface LDOS ressembles the (100) V surface LDOS. To the extend in which this LDOS is responsible for magnetism in this surface, the V side interface could be found be magnetic as well. This has important consequences in the interpretation of the superconducting tunelling experiments.

INTRODUCTION

The study of the physical properties of metal interfaces is gainning interest since almost ideal ones have become available experimentally. A deep understanding of such systems is crucial to the accurate description of superlattices and quantum wells whose practical applications are very wide.

THEORY

In this work we present a description of the V-Ta interface oriented in the (100) direction using the Green's Function Matching Method in the form cast recently by García-Moliner and V. Velasco [1]. This method makes use of the transfer matrices first introduced by Yndurain and Falicov [2] and is closely related with the decimation technique first formulated by Guinea et. al. [3]. The corresponding interface Green's function, G_I, is given by:

$$G_I^{-1} = G_{S(A)}^{-1} + G_{S(B)}^{-1} - J_A H^x J_B - J_B H^x J_A \qquad (1)$$

where $G_{S(A)}$ and $G_{S(A)}$ are the surface Green's functions for the semi-infinite media A and B, respectively. The last two terms take care of the matching of both surfaces to build an interface. The surface Green's function can be calculated from the formula:

$$G_s = (W - H)_{00} - H_{01} T \qquad (2)$$

where $W = \omega 1$ is the energy and 1 is a unit matrix. We use the customary description in terms of principal layers. A principal layer is defined as the number of atomic layers grouped is such a way that there is only nearest neighbours interaction between them. To project a Hamiltonian into a principal layer is to take the matrix elements of it within wave functions that describe the corresponding principal layer. One can use a linear combination of atomic orbitals (a base) located on each of the atoms of the atomic layers involved in the principal layer. In our calculation we will use the five orbitals with the symmetry of the d-band and we will neglect the less important s-band. Our principal layers are formed by two atomic layers and the tight-binding description [4] of the interactions goes up to second-nearest neighbours. Our tight-binding parameters reproduce very reasonably the bulk d-bands. In formula (2) H_{00} is a hamiltonian projected at the first principal layer and H_{01} is the matrix element between the first and second principal layers. T is the transfer matrix. It can be calculated from the knowledge of the hamiltonians described above using the quickly converging method proposed by López-Sancho et al. [5] and later

developed further by Baquero [6]. The Local Density of States (LDOS), $N(\omega)$, can be readily obtained from the usual formula:

$$N(\omega) = -\frac{1}{\pi} \text{Tr Im } G(\omega) \qquad (3)$$

A more comprehensive explanation of the method can be found in reference 7 and 8.

RESULTS

A. SURFACES: In Fig. 1 we present the LDOS at the surface, first and second atomic layer, respectively, and at a bulk atomic layer for Ta(100). The bandwidth at the surface layer shrinks about 1 eV. This known effect is due to the bulk. The origin in this figure is at the Fermi level, E_F. Charge neutrality has been taken into account by rigidly shifting the curve so that the right number of occupied states is obtained. The density of electron states per spin, $N(E)$, at E_F increases at the surface compared to the bulk by about 30%. This change in the LDOS at E_F that accours in the surface layer has an important influence in its specific physical behavior as in problems of catalysis, for example. In going into the bulk, the LDOS takes quickly the shape of the bulk LDOS as can also be seen in Fig. 1 showing that the surface effect is very localized. The Ta(100) surface at room temperature behaves like an ideal (bulk terminated) surface [9]. We have made the assumption that the surface is ideal in building up our hamiltonians.

In Fig. 2, we presented the V(100) surface. Again we have considered an ideal surface. The LDOS at the surface layer shrinks a little more, with respect to the bulk, compared to the Ta(100) case just discussed. Also it is more intense around the Fermi level E_F. The population at E_F is substantially bigger. We have not considered any s-d transfer. It is believed that there is about 0.7 electrons/atom/spin charge transfer to the d band [10]. If one take into account the s-d transfer just mentioned the highest accupied state would shift up in energy increasing substantially the number of electrons with this energy at the surface layer (see Fig.2). This enhancement of $N(E_F)$ is believed to be directly associated with the known magnetic properties [11] of the V(100) surface. This surface has been shown experimentally [12] to be magnetic although bulk vanadium is paramagnetic. The effect is quite localized as can be seen again in Fig. 2. The bulk LDOS appears also in this figure for comparison.

B. INTERFACE: We now consider the effect of matching these two surfaces to build up an interface. We calculated the interface Fermi level in the way proposed by Bonnelle et. al. [13], i.e., within the zero charge transfer approximation assuming that the matrix elements of the Contact Potential take its limiting values right at the first atomic layers forming the interface [8]. The interface tight-binding parameters were taken as the arithmetical average of the bulk ones. Since there are no experiments on this interface, it is not possible to check the validity of this assumption. It is nevertheless a very reasonable and widely used one and a natural point to start from. Any correction to this assumption is to be done on the basis of a detailed experimental analysis of the situation. Further, we have taken into account charge transfer at each atomic layer. The lattice constant of V is 3.03 Å while the one of Ta is 3.3 Å. This 10% mismatch will cause stress right at the interface. We did not take it into account in our calculation but - as we will explain below - our conclusions could be qualitatively the same.

In Fig. 3 we present the LDOS, $N(\omega)$, at the interface (zeroth layer), on the first and on a bulk atomic layer. There is not to much variation in the $N(E_F)$ as one enters into the material in tantalum. $N(E_F)$ is nevertheless smaller at the interface than at the surface (0.51 compared to 0.61 states/atom/spin/eV) but very similar to the bulk value (0.53). Actually the shape of $N(\omega)$ ressambles to the one of a bulk atomic layer much more than a surface atomic layer. The shape of this curve around E_F tells us about the influence that transfer of charge of any origen might do. We do not expect an important transfer of charge comming from the other side of the interface following the results of Ferrante et. al. [14] who showed that this effect is negligable in a wide variaty of metallic interfaces. But a certain band transfer can be expected (s-d). Nevertheless as $N(\omega)$ is almost flat around the Fermi energy, the effect of such a transfer will not cause any important changes at the tantalum side of the interface as long as the rigid band approximation remains valid.

As it is shown in Fig. 3, although different for the interface and the bulk the LDOS curve relaxes smoothly to the shape it has for a bulk atomic layer as one enters into any of the materials. The real sharp discontinuity occours right at the interface in going from one medium to the other.

A very interesting situation arises in the vanadium side. The first thing to notice in contrast with what we have first mention for tantalum is that the ILDOS curve is very similar to the SLDOS not to hte BLDOS. Further, the $N(E_F)$ is 0.73 states/atom/spin/eV in a bulk atomic layer while at the interface is 1.26 even higher than at the surface where it is about 1.0. The high number of electrons at the Fermi level in a surface layer was shown to be associated with the magnetic behavior of the V(100) surface first by G. Allan [11] and demonstrated experimentally by Rau et al [12]. This bring the idea that this interface could behave in a similar way as the surface does. If this is the case - as our results seems to indicate - the V-Ta interface could be magnetic although bulk metals are paramagnetic. If this turns out to be true one would wonder if, in general, the vanadium side of an interface would be magnetic. This takes us back to the old problem of the influence of paramagnons [15] on the I vs V charactheristics of a normal metal-oxide-vanadium tunelling junction from which the Eliashberg function of conventional superconductivity is determined. The question is then if a V-oxide interface will or will not be magnetic and if this atomic layer could act as a magnetic impurity in those experiments. Trying to stablish if this property is particular of vanadium we have also studied the V-Nb interface and found it to be again magnetic. It is necessary to calculate the V-oxide interface explicitly to arise at a solid conclusion but we would like to rise here the point abount the possibility that this particular behavior of a vanadium interface is at the basis of the unsettled problem of the influence of paramagnons on the I vs V characterisctic of superconducting vanadium.

CONCLUSIONS

We have studied the V-Ta interface by the Green's function matching method [1] using tight-binding hamiltonians in the orthogonal approximation and using a five-d-orbitals base on each atom in the language of Slater and Koster [4] and using the quickly converging algorithms of López-Sancho et al [5] as reviewed by Baquero [6] to calculate the transfer matrices. We have fixed the interface Fermi level following Bonnelle et al [13] which amounts to use the zero charge approximation with the assumption that the Contact Potential assumes its limiting values right at the first atomic layer on each side of the interface.

Our main result is that while in the tantalum side the inferface behaves essentially as a bulk atomic layer, in the vanadium side the interface behaves much more like a surface layer. Even more, $N(E_F)$ for the interface is higher than for the surface. Since this are important characteristics used by Allan to determine that the V(100) surface is magnetic, we suggest that the V-Ta (100) interface at its vanadium side might be magnetic as well. This an interesting result in itself but it can also be of importance in the explanation of the possible magnetic influence found in the I vs V characteristics of superconducting vanadium and commonly attributed to paramagnons [15].

REFERENCES

1- F. García-Moliner and V. Velasco, Progress in surface science 21, 93 (1986).
2- L.M. Falicov and F. Yndurain, J.Phys. C8, 147 (1975).
3- F. Guinea, C. Tejedor, F. Flores and E. Louis, Phys. Rev. B28, 4397 (1983).
4- J.C. Slater and G.F. Koster, Phys. Rev. 94, 498 (1954), W.A. Harrison, Electronic Structure and the Properties of Solids, W.H. Freeman, editor, 1980.
5- M.P. López-Sancho, J.M. López-Sancho and J. Rubio, J. Phys. F: Met. Phys. 15, 95 (1985).
6- R. Baquero ICTP-preprint IC/88/185.
7- R. Baquero, V. Velasco and F. García-Moliner, Phys. Scripta 38, 742 (1988).
8- R. Baquero, A. Noguera, A. Camacho and L. Quiroga, Phys. Rev. B (accepted).
9- R.A. Bartynski and T. Gustafsson, Phys. Rev. B35, 939 (1987).
10-R. Baquero, A. Camacho, L. Quiroga, Can. Jour. Phys. 67, 841 (1989).
11-G. Allan, Phys. Rev. B19, 4774 (1979).
12-C. Rau, C. Liu, A. Schmalzbauer and G. Xing, Phys. Rev. Letters 57, 2311 (1986).
13-C. Bonnelle, F. Cyrot-Lackmann, P. Jounard, J.P. Julian, D. Mayon and F. Vergand, Phys. Scripta 38, 100 (1988).
14-J. Ferrante and J.R. Smith, Phys. Rev. B31, 3427 (1985).
15-R. Baquero, J.M. Daams and J.P. Carbotte, J. Low Temp. Phys. 42, 585 (1981).

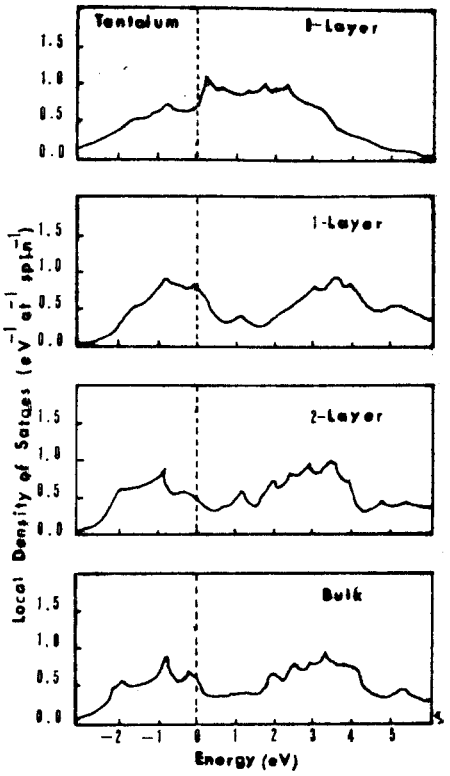

Figure 1. LDOS in the successive atomic layers on moving from the surface into the bulk for Ta(100).

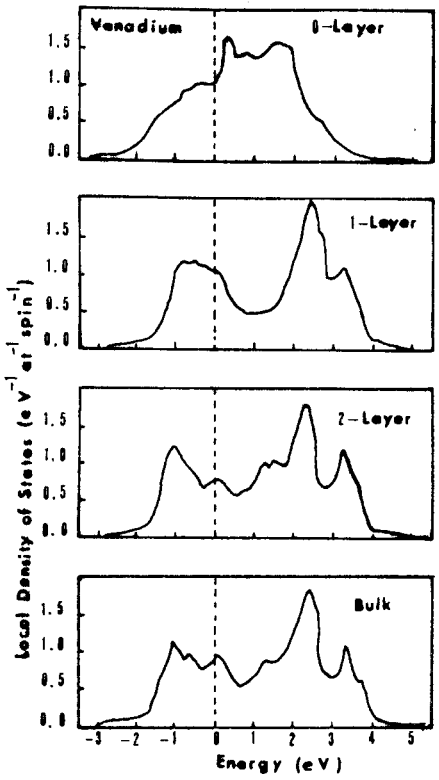

Figure 2. LDOS in the successive atomic layers on moving from the surface into the bulk for V(100).

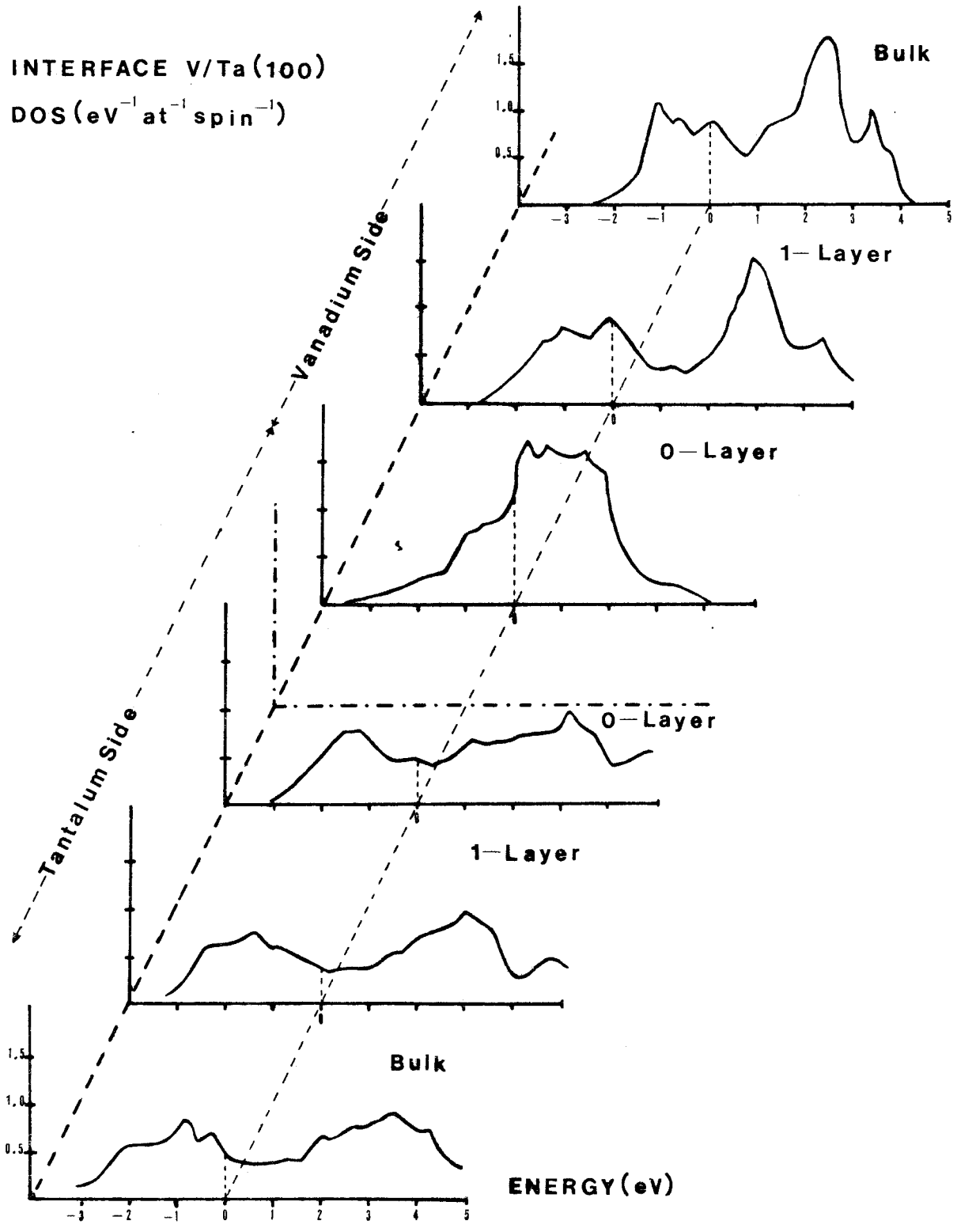

Figure 3. Evolution of the Density of States (DOS) for both sides of the V-Ta interface.