ELECTRONIC LOCAL DENSITY OF STATES FOR THE Mo/Ta INTERFACE

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We have calculated the interface local density of states (ILDOS) formed by the transition metals Mo/Ta using a tight=binding Slater-Koster description and the Green's Function matching method together with quickly converging algorithms to compute the transfer matrices. We obtain the surfaces LDOS as a byproduct. Our result is a useful tool to analyze experimental results and to check models as a function of the value of the tight-binding parameters either of the bulk or at the interface itself. We consider the (100) direction. We compare the interface to the bulk and to the surface and comment on some recently found experimental results for this interface.

INTRODUCTION

The study of the physics of surfaces, interfaces and superlattices of transition metals is the object of a new and increasing interest nowadays. At the origin of the deep understanding of the experimental results on these systems is an accurate description of its electronic band structures and its phonon spectra. In this paper, we use an empirical tight-binding[1] description of the electronic structure of the transition metals Mo and Ta to calculate the ILDOS using the Green Function Matching Method[2]. Our study is analogous to the recent calculation by Baquero et al.[3] for other transition metals. The LDOS for the surfaces is obtained as a byproduct.

We consider ideal interfaces. This is not a limitation anymore for metallic systems. Recent advances in thin-film-deposition technology[4] have allowed the fabrication of overlayers on surfaces, interfaces and superlattices under more strict control of the parameters entering the process of production and samples with a high degree of structural coherence are now possible.

Metallic interfaces are relatively seldom studied. The electronic structure of the Ni-Al interface was recently studied experimentally by Bonnelle et al.[5] by electron stimulated X-ray emission spectroscopy and the results analyzed theoretically by the recursion method[6] using tight-binding hamiltonians. Farquhar and Inglesfield have calculated the interface electronic structure by the embedding method very recently.[7] A tight-binding analysis of the cohesive properties of this interface can be found in Ref. 8. Also, the growth and modification of the Al/Ta(110) interface was studied by photoemission.[9] There is no previous study of the Mo/Ta interface known to us.

Artificially prepared superlattices of transition metals are a relatively new class of materials and their electronic, magnetic and superconducting properties are being studied quite intensively.[10] The Mo-Ta superlattice has been studied recently.[11]

II THE METHOD

As stated above, to describe the interface between two transition metals we make use of empirical tight-binding hamiltonians. Since the Green's function matching method takes into account of the perturbation caused by the surface or the interface exactly, at least in principle, we can use the tight binding parameters for the bulk. Their difference is taken into account through the matching of the Green's functions. We use the method in the form cast recently by García-Moliner and Velasco.[2] They make use of the transfer matrix approach first introduced by Falicov and Yndurain[12]. This approach became very useful due to the quickly converging algorithms of López-Sancho et al.[13] Following the suggestions of these authors, the algorithms for all transfer matrices needed to deal with surfaces, interfaces, quantum wells and superlattices can be found in a straightforward way.[14] The mathematical details of the method are described in references 2, 3 and 15. We will not discuss here them any further.

III RESULTS AND DISCUSSION

This is the first calculation of the interface Local density of states (ILDOS) for the Mo/Ta interfaces.

In Figs. 1 and 2, we show our result for the ILDOS. These were obtained with a two center, orthogonal empirical tight-binding description of the s,p and d-bands. The tight-binding parameters were taken from the work of Papaconstantopoulos.[16]

In Fig.1 we can see the LLSOS projected at the interface on the Ta atomic layer compared to the

surface and bulk LDOS. In Fig. 2, we present the analogous result for the projection on the Mo side.

In general, The bulk LDOS (BLDOS) for the bcc elements shows to peaks separated by a minimum. The Fermi level, E_F, is found usually around this minimum. The surface LDOS (SLDOS), in contrast presents a very strong peak around the position of the minimum in the BLDOS. The surface becomes very active when E_F occurs around the maximum in the SLDOS. The states at these energies for transition metals are predominantly d-like and are therefore very localized. This fact can lead tp special properties of transition metal surfaces. A known general characteristic of these LDOS is that the width of the bands is approximately the same for the interface and the bulk but for the surface it is narrower.

Let us concentrate on Fig. 1. where the Ta side of the ILDOS is compared to the BLDOS and SLDOS for Ta(100). Notice first that the general characteristics mentioned above hold for this case. The BLDOS presents two peaks of high intensity and two minor ones at the lower and higher energies respectively. The Fermi level occurs below the minimum in the BLDOS. The SLDOS is very different from the bulk and from the ILDOS. The two high maxima come closer to each other and the Fermi levels occurs in the quickly varying part of the spectrum showing that any charge transfer of whatever origin to this surface can change its properties. This can occur when overlayers are glown onto the surface. The ILDOS, the new result, turns out to be quite similar to the BLDOS but the Fermi level occupation is quite higher. Sometimes, interfaces have characteristics similar to surfaces of the same material. This does not seem to be the case for this interface.

Our figures have their origin at the Fermi level. When the bottom of the s band is taken as the origin, the values for E_F are for the tantalum side: 11.1 for the surfac, 9.4 for the bulk and 9.6 for the interface in eV.

In order to keep the highest energy level at the same energy on both sides we have added to the diagonal matrix elements of the hamiltonian in the Ta side, 0.8 eV following the procedure of Refs. 3 and 5.

Let us now concentrate in Fig. 2. The first thing to notice is that the ILDOS resembles the BLDOS again which is not the general case. When looking carefully we see that the Mo ILDOS is slightly shifted towards higher values of the energy. The Fermi level is right at the minimum and therefore any charge transfer will have consequences in the behavior of the interfaces. The density of states at the Fermi level is quite lower on this side of the interface than on the other side. This is the real sharp discontinuity at the interface. The ILDOS in the Mo side resembles the BLDOS much more than the SLDOS and no similarities between the interface and surface behavior can be inferred from this results. The Mo(100) surface does reconstruct and it is believed that the surface states are responsible for it. The density of states at the Fermi level is very big for the surface case when compared to the bulk or the interface case. A last point concerns the Mo/Ta superlattice. In the study of the superconducting properties of this superlattice of Ref. 11. the superconducting critical temperature, Tc, of samples with different layer thicknesses, Λ ($d_1=d_2=\Lambda/2=d$) were measured. They have obtained a monotonical decrease of Tc with Λ which they could account for within the de Gennes-Werthamer theory[11,17] on the proximity effect in the region where d is larger or comparable to the superconducting coherence length, ξ. To fit the data at $d<\xi$ they needed an additional mechanisms reducing the intrinsic Tc of the superconductors. They have related this effect to the smearing of the density of states N(E) and a lowering of $N(E_F)$. It is interesting to notice in this respect that in our study of the Mo/Ta interface, we get a reduction of the Fermi level population with respect to the bulk value on both sides of the interface.

IV CONCLUSIONS

We have calculated the interface local density of states (ILDOS) for the transition metal interface Mo/Ta in the (100) direction by using an empirical tight-binding hamiltonian and the Greens function method matching to calculate the interface Green function.

As a general feature we get that the ILDOS in both sides of the interface looks similar as the bulk projected LDOS which is very different from the surface local density of states in the same direction. Also we get a local density of states at the Fermi level which is in both sides smaller than the bulk value. It is possible that this is related to the measured dependence of Tc with respect to Λ, the layer thickness of the superlattice.

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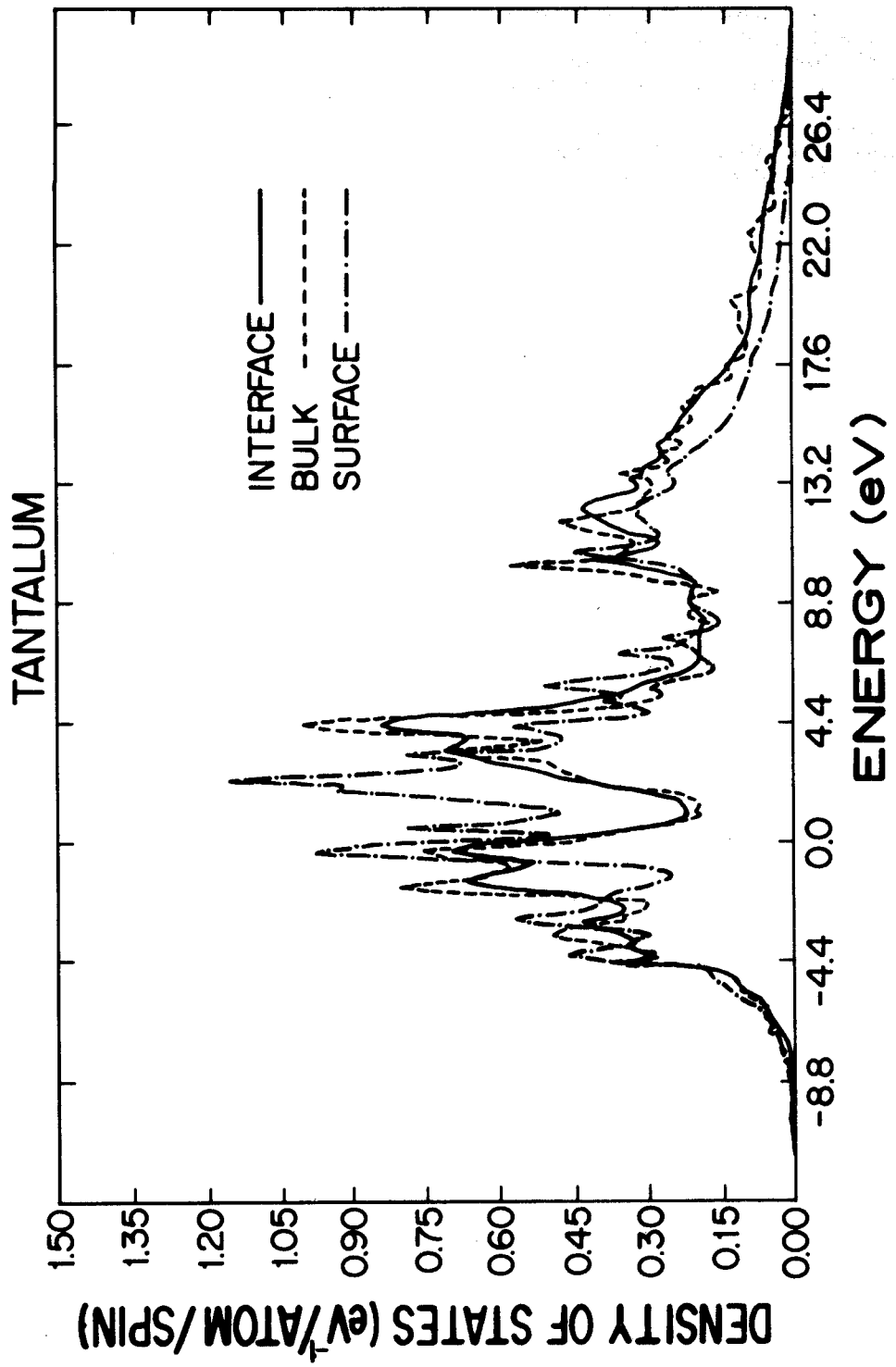

Fig. 1 The Tantalum side of the interface.

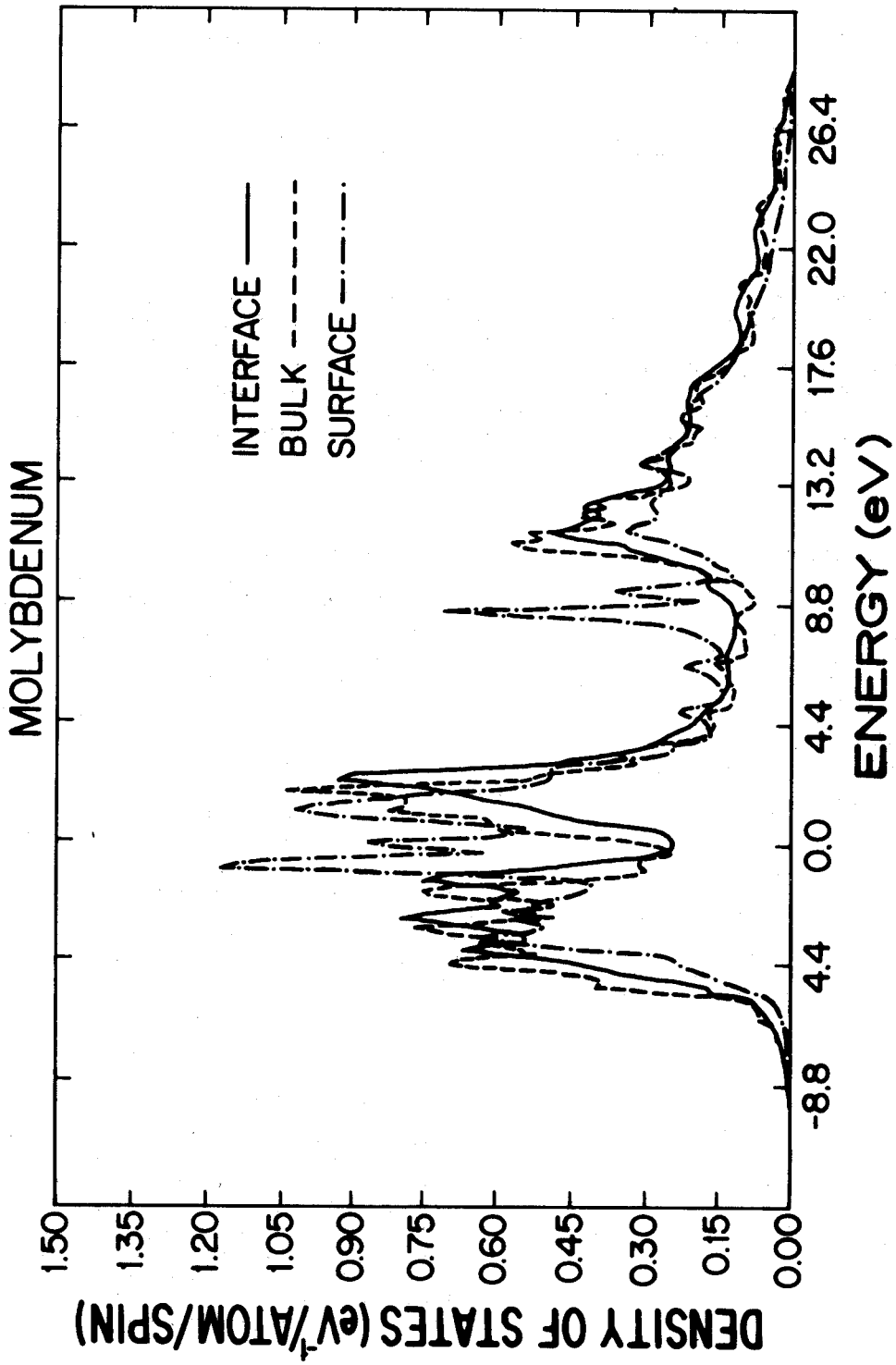

Fig. 2 The Molybdenum side of the interface.