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Local density of states for transition-metal interfaces

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We have calculated the interface local density of states (LDOS) for the three transition metals V, Nb, and 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 surface LDOS as a byproduct. The calculation turns out to be an almost trivial computational problem. The method proves to be a very 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 or as a function of different geometrical situations. It is also a solid basis on which other problems depending on a proper description of the local density of states can be worked out. We analyze in detail the Nb/Ta, Nb/V, and Ta/V interfaces in the [100] direction. We find that some of the properties found in surfaces could also be found at interfaces. In particular, we find that the V side of some interfaces could show magnetism on the atomic layer in contact with the foreign medium as the (100) surface does for this metal.

I. INTRODUCTION

The study of the physics of surfaces, interfaces, and superlattices of transition metals is drawing 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. The *ab initio* calculations are the most appropriate answer to this problem. Yet another method of calculation, which allows an easy and quick test of models, hypothesis, and geometrical situations, has proven desirable. There are several proposals in the literature for this alternative method. It is the purpose of this paper to illustrate the use of a very simple one that takes full advantage of the existing ingredients for the calculation of the electronic band structure (EBS) and local density of states (LDOS) for interfaces of transition metals. The LDOS for the surfaces is obtained as a byproduct. The method can be applied to superlattices as well. Phonons can also be treated in this way. We will consider the three metals V, Nb, and Ta, as a specific example.

In the past, most of the work on mesoscopic systems was concentrated on semiconductor-semiconductor and metal-semiconductor heterojunctions.[1] The work on artificially layered metals was initiated long ago and was aimed at producing layered structures for x-ray diffraction gratings and polarizers and monochromators for neutrons. It was discovered early on that interdiffusion greatly affected the structures produced and many workers have concentrated on these materials for the study of the physics of diffusion. In our work we consider ideal interfaces. This is not a limitation. Recent advances in thin-film-deposition technology[2] have allowed the fabrication of overlayers on surfaces, interfaces, and superlattices under stricter control of the parameters entering the process of production, and samples with a high degree of structural coherence are now possible. These artifically prepared materials are of great interest since they can exhibit properties different from those that occur in nature. Nevertheless, a minimum perfection in the growth of the sample is to be achieved before these properties manifest themselves. For example, superlattices will not exhibit their specific electronic properties unless interdiffusion between the two media is avoided to a great extent.[2]

The electronic structure of metallic surfaces was extensively studied[3] as well as their magnetic properties.[4] Our work is useful as a solid starting point for the theoretical description of problems, such as the enhanced magnetic moment that some surfaces exhibit with respect to the bulk, as in the Fe(001) (Ref. 5) and the Ni(001) (Ref. 6) surface, or the temperature dependence of magnetization on surfaces. Reconstruction and its temperature dependence is another problem of interest. For example, the temperature-dependent reconstruction of the W(001) surface[7] seems to have its origin in the occupation of surface states very close to the Fermi level and therefore requires a careful description and study of these levels. Several metallic surfaces are under study concerning hydrogen adsorption.[8] Efforts have also been devoted to the catalytic activity of surfaces. One focus of interest is the influence of overlayers. Sometimes a few atomic layers on a given surface[9] are enough to produce important changes in the catalytic rate of some reactions. The temperature dependence of magnetization of surfaces and the influences of overlayers on it have been described by Hasegawa[10] on the basis of an electronic LDOS calculated with a method similar to this, although we take full advantage of the use of transfer matrices.

Metallic interfaces are studied less than surfaces. Although interesting in themselves, the deep understanding of the physics of the interface is an important starting point for the detailed study of superlattices. The electronic properties at solid-solid interfaces depend sometimes even on details of the interaction between the two atomic layers from the different materials in contact. Our work can be used as a starting point to analyze those details. These are responsible for the characteristics of the interface: reconstruction, thermodynamic properties, degree of intermixing, stress, compound formation, etc.

The electronic structure of the Ni/Al interface was recently studied experimentally by Bonnelle *et al.*[11] by electron-stimulated x-ray emission spectroscopy, and the results were analyzed theoretically by the recursion method[12] using tight-binding Hamiltonians. Very recently, the growth and modification of the Al/Ta(110) interface was studied by photoemission.[13] There is no previous study of the interfaces that we consider here.

Artifically prepared superlattices of transition metals are a relatively new class of materials, and their electronic, magnetic, and superconducting properties are being studied quite intensively.[14] The Nb-Cu superlattices are among those studied more frequently.[15] Other transition-metal superlattices that have drawn attention are the Nb-Ti,[16] Cu-Ni,[17], Pd-Ni,[18] V-Ni,[19] Mo-Ni,[20] V-Ag,[21] and, more recently, Mo-Ta.[22] The rest of our paper is organized as follows. In Sec. II we present the method of calculation used. The results and discussion appear in Sec. III and our conclusions are presented in Sec. IV.

II. METHOD

To describe the interface between two transition metals, we make use of tight-binding Hamiltonians. Since the Green's-function-matching method takes into account the perturbation caused by the surface or the interface exactly, at least in principle, we can use the tight-binding parameters for the bulk. This does not mean that we are using the same tight-binding parameters for the surface, or for the interface and the bulk. Their difference is taken into account through the matching of the Green's functions. The first work on the decimation technique was done by Guina *et al.*[23] We use the method in the form cast recently by García-Moliner and Velasco.[24] They make use of the transfer-matrix approach first introduced by Falicov and Yndurain.[25] This approach became very useful due to the quickly converging algorithms of López-Sancho *et al.*[26] Following the suggestions of these authors, the algorithms for all transfer matrices needed to deal with mesoscopic systems can be found in a straightforward way.[27] This method has been employed successfully for the description of surfaces.[28] Since the bulk tight-binding parameters for numerous solid elements are now available from the recent work of Papaconstantopoulos,[29] this work illustrates a practical and systematic way to describe the electronic LDOS of mesoscopic systems.

The mathematical details of the method are described in Ref. 24. We will discuss here some complementary aspects. To set the Hamiltonian one can use the two- or three-center orthogonal approximation within the language of Slater and Koster.[30] The use of an orthogonal basis is not a necessary limitation. One can also use a nonorthogonal one. It is also possible to use a *d*-band description, an *s*-*d*-band description, or an *s*-*p*-*d*-band one according to the specific nature of the problem and the degree of computational simplification desired. The corresponding tight-binding parameters have to be found for each case. The values for the *s*-*p*-*d* tight-binding parameters are given in Ref. 29. In the same work the values of the energy at the high-symmetry points of the three-dimensional (3D) first Brillouin zone are also given. With these data and the form of the bulk Hamiltonian it is not difficult to set a system of equations at the high-symmetry points to find the tight-binding parameters. For the *d*-band case, a formula is also given by Harrison.[31]

In our description of transition-metal interfaces we have assumed ideal truncation, as commented above. Nevertheless, the same method can be used to describe intermixing at the interface to the degree in which the tight-binding parameters of an element can be extended to a compound. Also, stress can be taken into account by using the d^2 scaling law of Harrison.[31]

Finally, we want to point out the usefulness of this description in the theoretical interpretation of experimental results, since it is very easy to play with the tight-binding parameters to clarify the source of a particular behavior.

III. RESULTS AND DISCUSSION

This is the first calculation of the interface local density of states (ILDOS) for the transition metals considered here.

In Fig. 1, we show the interface LDOS (ILDOS) for the three cases. These were obtained with a two-center, orthogonal tight-binding description of the *d* bands. In Fig. 2, we show a typical result with an *s*-*p*-*d* basis for comparison. It is clear that a meaningful description of the interfaces can already be obtained using just a *d* basis, since those states are the ones that contribute by far the most. This might be the simplest possible description of the problem and turns out to be computationally trivial. We show in Table I the tight-binding parameters used. They give a very reasonable description of the bulk *d* bands for the three metals. In any standard computer the analysis of models for the interface by changing the tight-binding parameters or the geometrical situation can be due interactively in most cases. This is a nice advantage of this formulation.

In Fig. 1 we can see the evolution of the LDOS as one enters into the bulk in both sides of the interface. The zeroth layer is the atomic layer in contact with the foreign medium. We show the bulk LDOS (BLDOS) for both media to compare with. We have also calculated the LDOS projected at the first atomic layer. As expected, its shape is somewhere in between the zeroth atomic layer and the bulk. The LDOS varies "smoothly" from its shape at the interface to that of the bulk as one goes into the medium. Therefore, even if the BLDOS and the ILDOS in a given medium differ substantially, the real sharp change in the LDOS in the nearest-neighbors scale is in going from one side of the interface to the other one. There is a region where these sharp changes still manifest themselves into the bulk in both sides which might be called the interface dominion. This is typically three to four atomic layers thick on each side of the interface. From this distance onwards the physical parameters that characterize the atomic layers are the ones of the bulk.

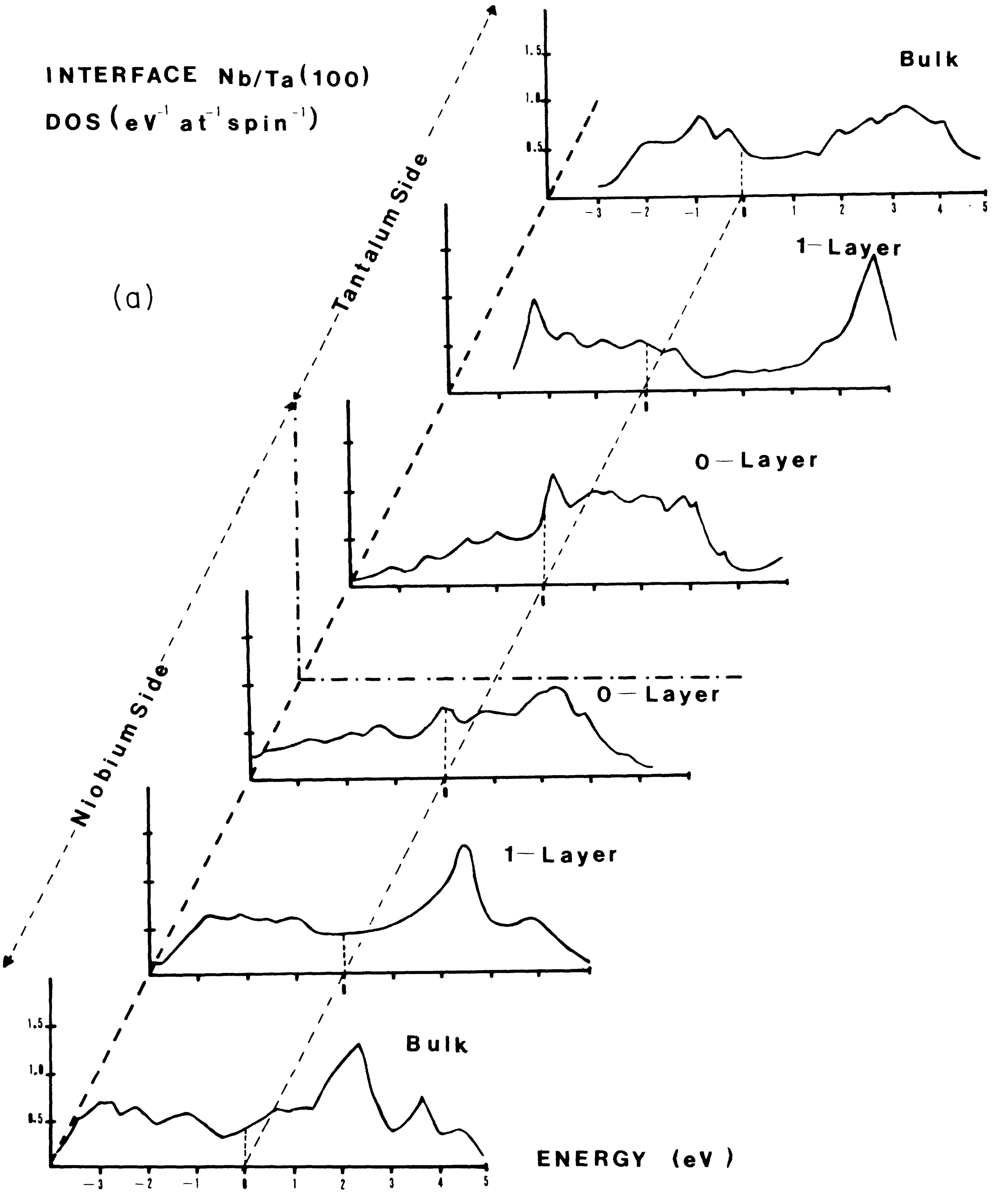

FIG. 1. Evolution of the density of states (DOS) for both sides of (a) the Nb/Ta interface, (b) the Nb/V interface, and (c) the V/Ta interface.

In Fig. 3 we give a detailed account of the behavior of each face of the interface for the cases considered and compare it to the corresponding free-surface LDOS (SLDOS) and to the BLDOS. The SLDOS and the BLDOS are quite different from each other. The observed bandwidth shrinkage for the surface is attributed to the lower number of nearest neighbors. This effect is missing at an interface, as can be seen in the same figure. The LDOS at the Fermi level differs sometimes for the bulk, the surface, and the interface for the three metals.

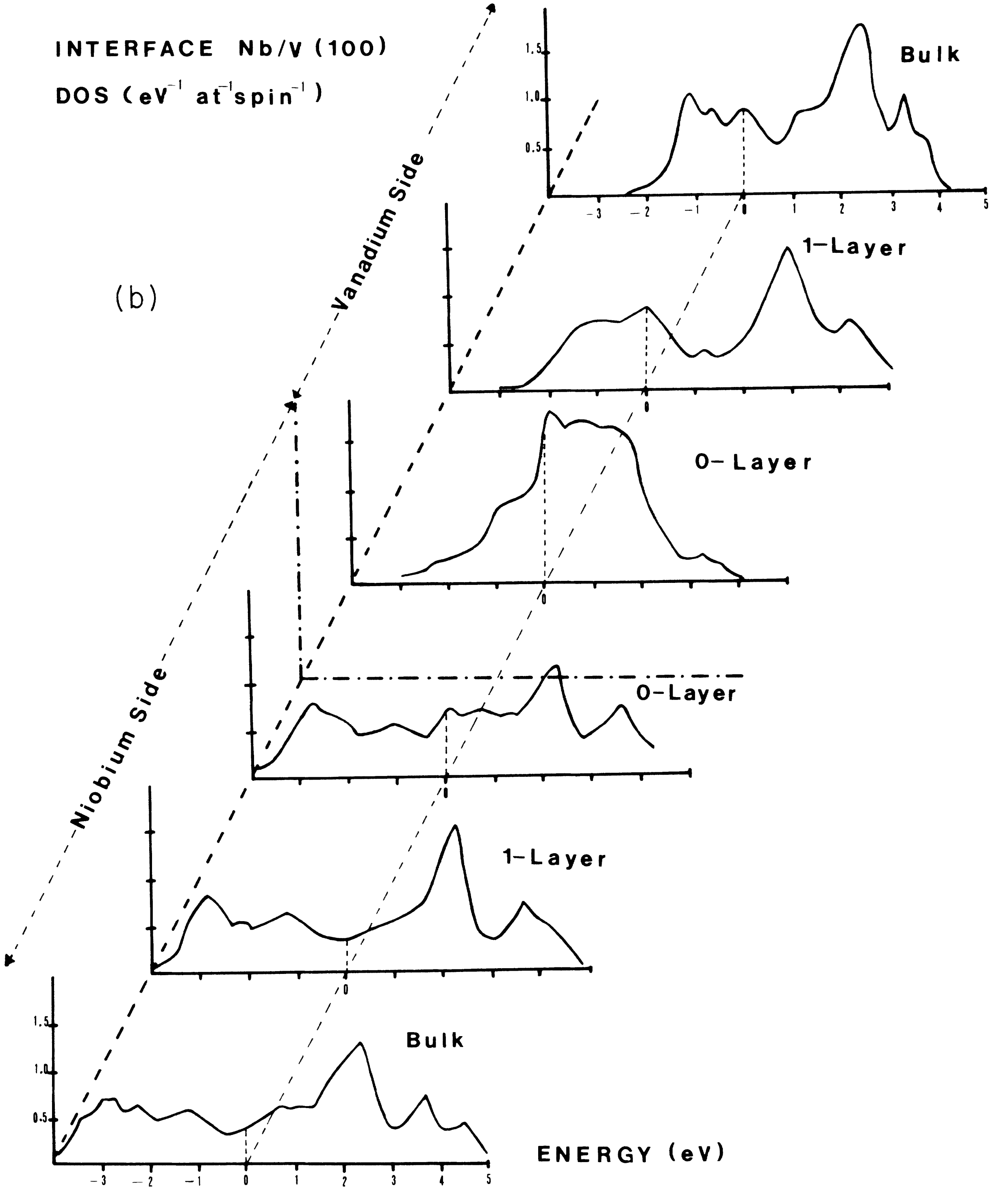

FIG. 1. (*Continued*).

This explains, for example, that the surface behaves sometimes very differently compared with the bulk and might point to some physical characteristics to be expected from particular interfaces (see below). In Table II, we give the Fermi-level density of states in all cases, for comparison. In metallic surfaces, the enhancement of the Fermi-level density of states is sometimes associated[31] with the loss of "places for an electron to jump to." This makes the electron "spend more time" around an atom at the surface than in the bulk. This argument cannot be

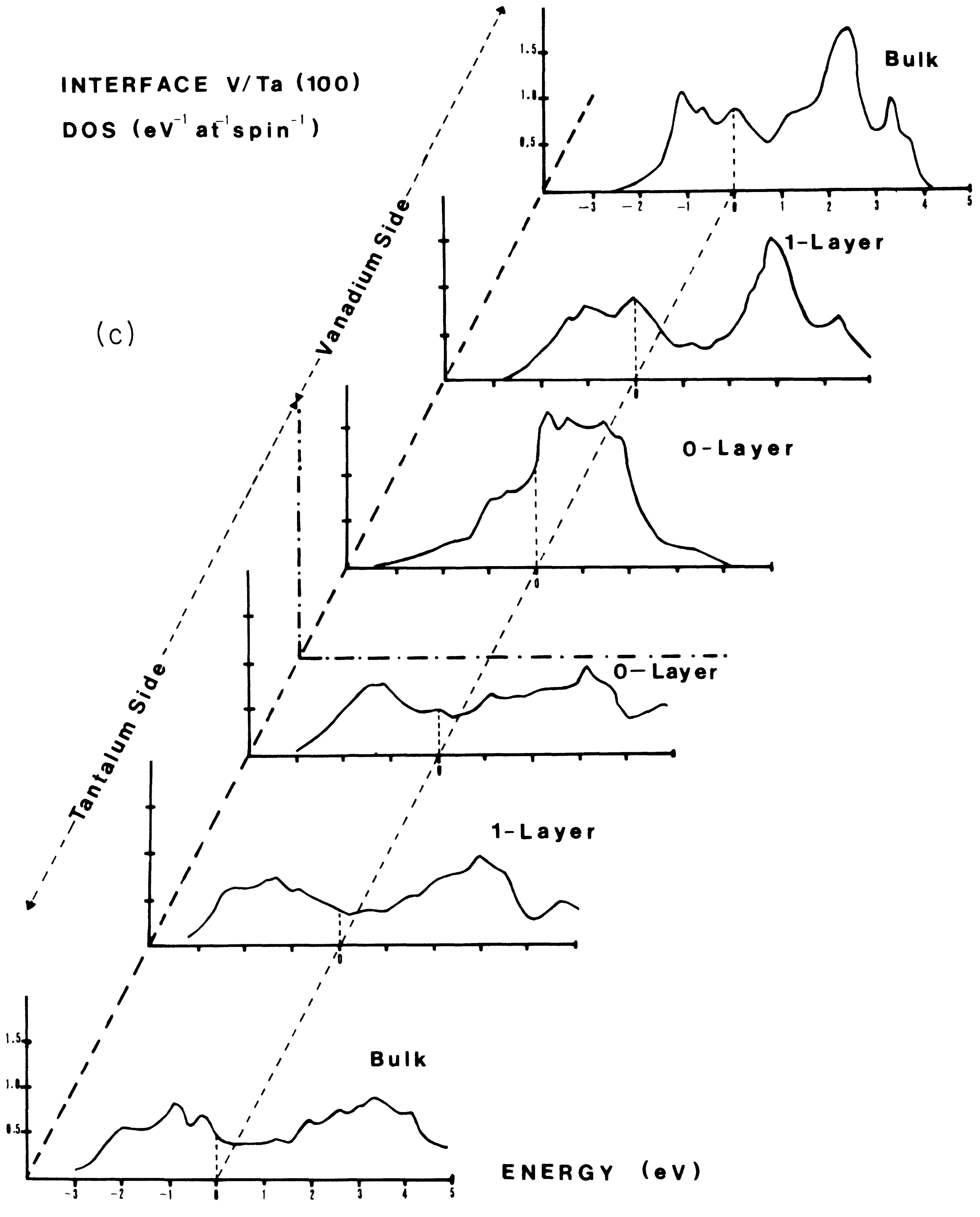

FIG. 1. (*Continued*).

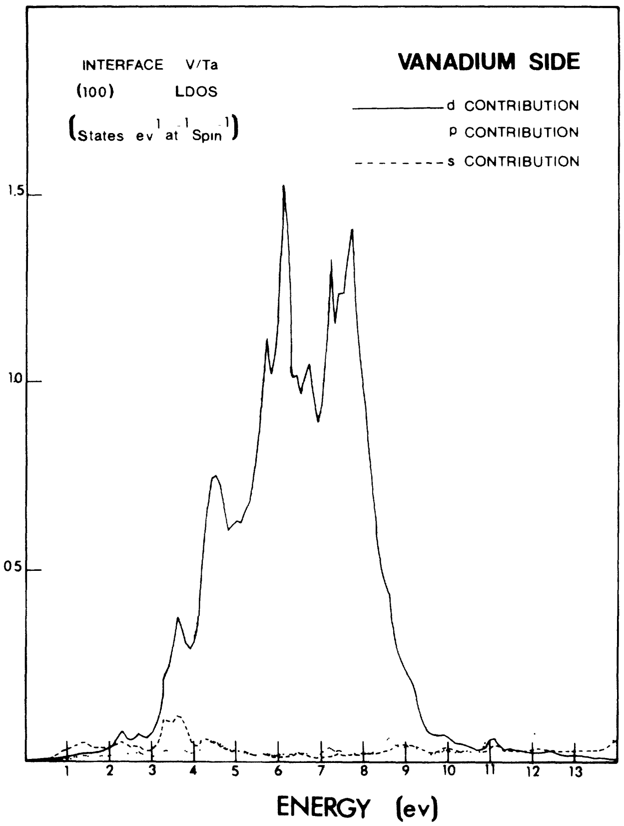

FIG. 2. Contribution of the s, p, and d bands to the V ILDOS.

used at the interface. Here the reason is to be attributed to specific details of the crystal potential there and a general trend is not to be expected. We will comment on each interface in more detail below. Let us deal with the calculation of the Fermi level first.

A. The Fermi level

The origin of the energy scale in all our figures is at the Fermi level E_F. We have fixed it starting from the bulk one for each material, $E_F^{(A)}$ and $E_F^{(B)}$, respectively, which we have calculated by integrating the corresponding bulk LDOS, $N_{\text{bulk}}(w)$, to get the total electron occupation per atom per spin, n_0, from the usual equation:

$$n_0=\int_{-\infty}^{E_F} N_{\text{bulk}}(\omega)d\omega \ . \tag{1}$$

The electron occupation per atom, per spin, n_0, decomposes into the s, p, and d contributions, as shown in Fig. 2. When one does not wish to describe all the bands occupied up to the Fermi level, but only some of them, the possibility of interband charge transfer within the same medium has to be taken into account.[32] This can be taken from the work (bulk) of Papaconstantopoulos.[29] On the other hand, the interband charge transfer might differ at the surface or interface from that of the bulk. For example, from considerations on the magnetic behavior of the V(100) surface, it was found[33] that 0.7 electron/atom spin could be a reasonable value for the surface s-d charge transfer in this case. The two values differ slightly. Otherwise, if we want to remain strictly within a d-band description, we can just take n_0 to be the atomic nominal d occupation. This procedure neglects interband charge transfer. We have considered both possibilities. They differ consequently. Our figures show the results for this last option. To fix the Fermi level E_F at the interface, we have followed exactly the procedure used in Ref. 11, i.e., we have taken the zero of energy at the common work-function position and ensure that the highest occupied level is the same in both sides of the interface by adding a potential equal to the difference in the Fermi-level energies to the side with the lowest E_F. Since all three metals have about the same work function (about 4 eV), the method used by Bonelle *et al.* to determine E_F turns out to be quite accurate in this case. Furthermore, we took into account charge neutrality at each atomic layer.

Finally, the Fermi level for the surface can be fixed from (1) using our calculated SLDOS and n_0.

TABLE I. The tight-binding parameters for the description of the d band. The corresponding ones for the s-p-d basis can be found in Ref. 28.

Parameter (eV)	Vanadium	Niobium	Tantalum
$(dd\sigma)_1$	-0.9035	-1.3783	-1.5813
$(dd\sigma)_2$	-0.4630	-0.6714	-0.7703
$(dd\pi)_1$	$+0.4958$	$+0.7444$	$+0.8541$
$(dd\pi)_2$	$+2.2124$	$+0.3626$	$+0.4161$
$(dd\delta)_1$	-0.0799	-0.1198	-0.1375
$(dd\delta)_2$	0.0	0.0	0.0
d_0	0.0	0.0	0.0

B. The Nb-Ta interface

Figure 1(a) shows the Nb/Ta interface. Since these two metals have the same lattice constant and the same crystallographic structure, there is no stress in this case. It is interesting to notice that the LDOS at E_F, $N(E_F)$, increases by almost 85% at the interface as compared to the bulk in Nb, while in the Ta side this effect is less than 40% and the LDOS at E_F oscillates slightly going through a minimum at the first atomic layer. Therefore, the difference in $N(E_F)$ at the interface compared to the bulk is much more important for Nb than in Ta.

The structure of the ILDOS is interesting to observe in more detail [see Figs. 3(a) and 3(b)]. On the scale of 0.5 eV around E_F the changes in the intensity of this curve are very different in the two sides. For Nb, the ILDOS is roughly symmetric and changes only up to about 10% of its value at E_F. In contrast, in the Ta face the ILDOS is a quickly increasing function of the energy and its value at the peak is more than twice that at the low-energy one. After the peak position it also decreases rapidly. Very near the Fermi level it is a very quickly increasing function of the energy. As a consequence, charge transfer will be important in this case since it could change drastically the Fermi level density of states. On the other hand, in the Nb side of the interface the effect of charge transfer would be much less important.

In this context, we recall that the W(001) surface (W is the element next to Ta in the Periodic Table, i.e., with one more electron) does reconstruct in a temperature-dependent way. This has been attributed to the occupation of surface electronic levels near E_F.[7,34] In the rigid band approximation the SLDOS would differ from the one we calculated for Ta only in the occupation of states at E_F [see Fig. 3(b)]. Thus, it might be possible that a behavior somehow related to this reconstruction is also observed in the W(001) side of a W/Nb interface. Furthermore, it is to be expected that an extra charge of whatever origin in the Ta(001) side of the Nb/Ta interface will cause important changes.

C. The Nb/V interface

This interface is shown in Fig. 1(b). The lattice constant of Nb is 3.3 Å while the one for V is just 3.03 Å. This is a stressed interface. Our results do neglect stress. We will comment on its effects below.

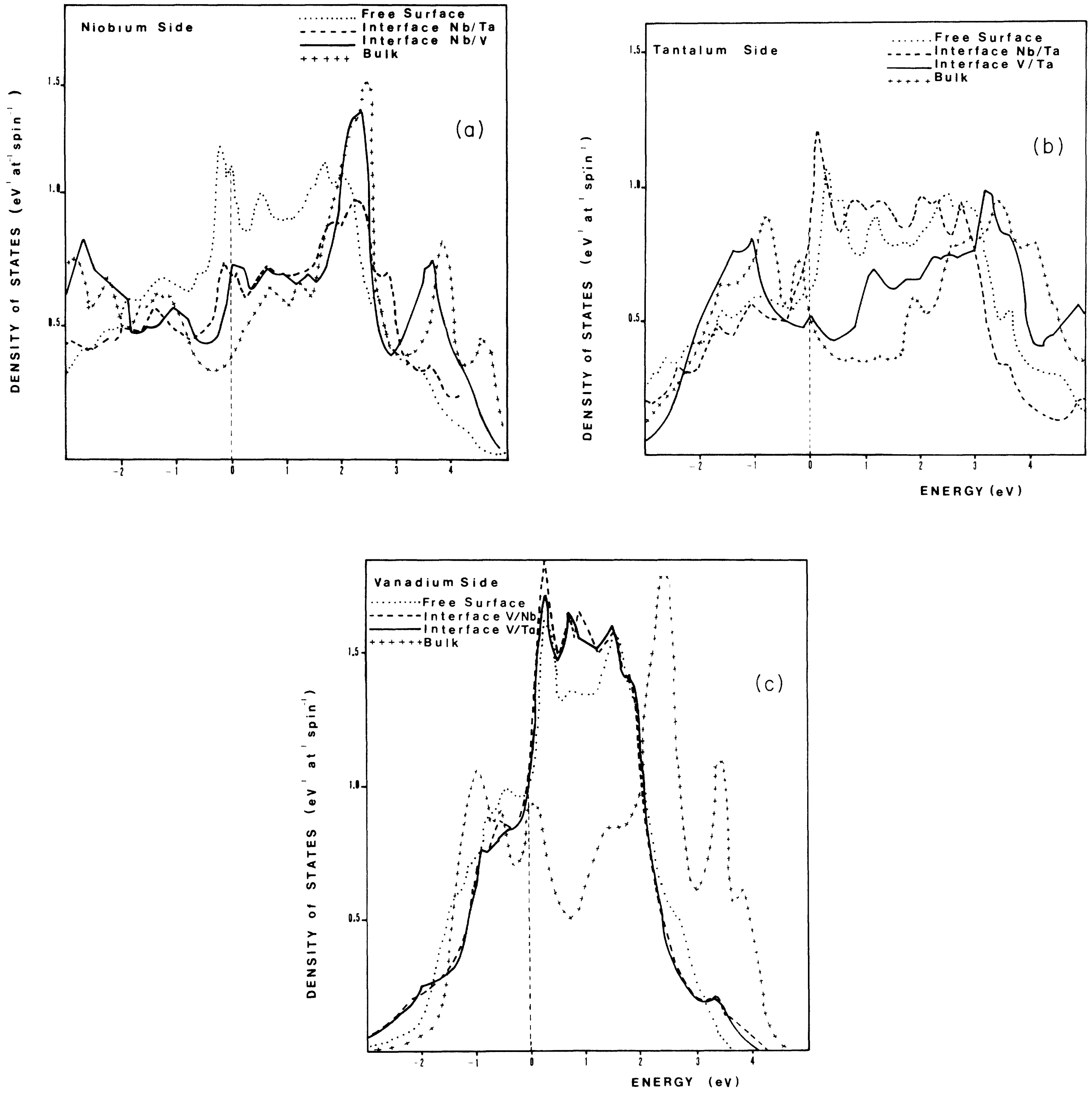

FIG. 3. The niobium SLDOS, BLDOS, and the ILDOS for Nb/Ta and Nb/V interfaces. (b) The tantalum SLDOS, BLDOS, and the ILDOS for Nb/Ta and V/Ta interfaces. (c) The vanadium SLDOS, BLDOS, and the ILDOS for Nb/V and V/Ta interfaces.

TABLE II. The calculated Fermi-level population is given for all cases considered. The [100] direction is meant when appropriate. For the V(100) surface and for the vanadium side of the two interfaces the value in parentheses is the one obtained by assuming a charge transfer of one electron per atom, per spin. Notice the important increase in the V(100) SLDOS and ILDOS for the Nb/V interface [see also Fig. 3(c)]. For the surface this effect is associated with magnetism. It is possible that, in general, the V side also shows magnetism in cases where its behavior is similar to the surface one as in Nb/V interface.

Interface	Niobium side	Vanadium side	Tantalum side
Nb/Ta	0.70		0.74
Nb/V	0.39	1.22 (1.62)	
V/Ta		0.126 (1.61)	0.51
Surface	1.07	1.0 (1.3)	0.61
Bulk	0.38	0.73	0.53

The same general remarks as in the previous case apply here. The ILDOS goes "smoothly" to the BLDOS as one goes into any of the two media so that the real sharp change occurs at the interface atomic layer. Here, $N(E_F)$ in Nb oscillates slightly when entering into the bulk. Notice from Fig. 3(a) that $N(E_F)$ is about the same at the two interfaces in the Nb side. A striking fact in this case is the sharp change in $N(E_F)$ that occurs right at the interface [see Fig. 1(b)]. $N(E_F)$ is more than three times bigger in the V side than in the Nb one. Notice that due to the shape of the LDOS curves near E_F, adding electrons at E_F will cause an important increase in $N(E_F)$ at the V side of the interface, while a very minor one at the Nb one. A further comment can be added if we examine Fig. 3(c). At the V side of this interface the electronic population, $N(E)$, around the Fermi level follows closely the SLDOS. Since the evolution into the bulk of the LDOS is very similar in the surface and the interface cases, a similar behavior can be expected. In particular, the V(001) surface has been shown experimentally to be magnetic.[35] A strong *s-d* transfer of at least 0.7 electron/atom spin is expected in the surface case.[33] If such a transfer also occurs in the interface case, the $N(E_F)$ would increase substantially, as can be seen in the same figure. Notice that at the V side of this interface the increase in $N(E_F)$ would be even slightly higher than in the surface. Since all relevant characteristics for magnetism seem to remain at least equally favorable in the interface and at the surface, one wonders if the V side of this interface shows a magnetic behavior as well. The inclusion of stress could change this conclusion for this particular case, but not the qualitative remark that some V(100) interfaces could also show magnetism. An interesting conclusion arises: magnetism could appear at the interface of two paramagnetic materials.

D. The V/Ta interface

In Fig. 1(c) we show finally the V/Ta interface. Since the lattice constant for Ta is about 3.3 Å (as for Nb), this is again a stressed interface. We did not take this effect into account.

For Ta, the variation of $N(E_F)$ as one enters the material is not very big. From Fig. 3(b), we can see that the LDOS curve does not vary very much around E_F for this interface. Consequently, this side of the interface might not change its behavior in the case of charge transfer of whatever origin. Right at the interface, the ILDOS more closely resembles the BLDOS than the SLDOS, in contrast with the Nb/Ta interface presented before, where the ILDOS follows closely the SLDOS. The $N(E_F)$ at the Ta side of the V/Ta interface is essentially the same as for the bulk, in agreement with the observation just made.

The V side is studied in Fig. 3(c). Here again, the ILDOS does follow the SLDOS quite closely. The $N(E_F)$ is essentially the same as for Nb/V presented before and the same observation about the effect of charge transfer applies. Again we expect magnetism in this case.

Finally, it is to be noticed that, as a general trend, the ILDOS at the V side of these interfaces has a shape that more closely resembles the SLDOS. The Nb side of the interfaces seem to be more like the BLDOS. Ta is an intermediate case in this sense.

We now make a final remark about the possible existence of V(100) magnetic interfaces. As it appears from this study, there is a real possibility that this interface could show magnetism. Nevertheless, the effect of stress is to be set. Since this is a qualitative study, we can decide about this effect only by stating that vanadium under stress (expansion) does become magnetic, as is mentioned in Ref. 36. Therefore, stress could even favor magnetism at the interfaces, and we conclude, therefore, by stating that this is a qualitative prediction of the existence of such an effect at some V(100) interfaces.

IV. CONCLUSIONS

In conclusion we have calculated the ILDOS for the three interfaces Nb/Ta, Nb/V, and V/Ta. We have used tight-binding Hamiltonians to describe the *d* bands of each transition metal. This very simple description of the problem turns out to be meaningful since these are the states that contribute the most to the ILDOS, as is shown in Fig. 2. The computational problem turns out to be trivial. This method allows the quick test of models that depend on the size of the tight-binding parameters (TBP) or on different geometrical situations, and should therefore be very useful to analyze experimental results.

We use the Green's-function-matching method in the recent formulation of García-Moliner and Velaso.[24] In this method the bulk TBP are to be used since the formulas take into account the perturbation caused by the interface explicitly and, in principle, exactly. Since the TBP for several elementary solids are now available, our work should be useful as a solid basis to deal with problems such as reconstruction, stress, catalysis, magnetism, interface superconductivity, temperature dependence of certain physical phenomena, etc.

The main conclusion of our paper is the possible existence of magnetic V(100) interfaces. We have arrived at it by showing that the parameters that enter in the two-dimensional Stoner criterion established by Allan[6] for surfaces are about the same for the V side of the studied interfaces. The same criterion can be applied to predict magnetism at these interface and allows us to conclude that at least some V(100) interfaces might show magnetism as does the V(100) surface.[6,35]

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