

Multilayer relaxation at surfaces of body-centered-cubic transition metals

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We present a calculation of the multilayer relaxation for six low-index surfaces of Nb, Ta, Mo, and W, based on the "quenched molecular-dynamics" approach, in which we minimize the total energy in a tight-binding framework. The six surfaces considered here are the (110), (100), and (111) faces, which present only perpendicular relaxations and the (211), (310), and (210) faces for which both parallel and perpendicular components are present. The profile of perpendicular relaxations is found to be face dependent but, contrary to that of parallel relaxations, roughly metal independent. These results are in good agreement with existing experiments.

I. INTRODUCTION

It is now well established that metal surfaces undergo relaxations (i.e., their layers of atoms are rigidly translated from their bulk positions; see Ref. 1 for a review). The experimental results are mainly obtained by low-energy electron diffraction¹ (LEED) and ion scattering studies.²

They show that multilayer relaxation is a rather common phenomenon and that the relaxation profile varies dramatically from one surface to one other. Moreover, for unsymmetrical surfaces (i.e., surfaces for which there does not exist at least two mirror planes) the relaxation would have parallel as well as perpendicular components.³⁻⁵

From a theoretical point of view Allan and Lannoo⁶ predicted a long time ago a contraction of the first interlayer distance using a second-moment approximation of the tight-binding scheme. The same model was used to study monolayer relaxations of the (100), (110), and (111) surfaces of fcc transition metals,⁷ the (100) surface of bcc Mo and W,⁸ and stepped surfaces of fcc transition metals.⁹ More recently some similar studies for low-index surfaces of bcc and fcc transition metals have been proposed.^{10,11}

Another approach is the electrostatic model of Finnis and Heine.¹² This model is only qualitative and Barnett *et al.*¹³ found that a reliable calculation must include an evaluation of the screening response of the conduction electrons to the relaxed ionic system. Moreover this work is only valid for simple metals. An empirical version of this model was very recently proposed by Jiang *et al.*^{14,15} (referred to as JJM in the following). These authors perform calculations for many fcc and bcc surfaces. The agreement with experimental results on Fe and Al is rather good. However, this empirical approach requires the knowledge of one parameter which is fitted to the experimental relaxations; it cannot predict the evolution of the relaxation from one metal to another in the absence of experimental results.

The last set of theoretical results comes from more *ab initio* methods. Unfortunately only a few surfaces were studied using such approaches: W(100),^{16,17} V(100),¹⁸ Ru(0001),¹⁹ and Al(110).^{20,21}

In the present work we calculate within the tight-binding scheme and use the "quenched-molecular-dynamics" method to find the multilayer relaxation of six surfaces, (110), (100), (111), (211), (310), and (210), for four nonmagnetic bcc transition metals Nb, Ta, Mo, and W. This allows us to characterize the relaxation profile (i.e., face, and metal dependence).

In Sec. II we summarize the method used for the calculations; in Sec. III we present the results for the symmetrical surfaces (where only perpendicular relaxations occur) and in Sec. IV the results for unsymmetrical surfaces (with both perpendicular and parallel components of the relaxation). Finally, in Sec. V our results are compared with previous calculations of multilayer relaxation.

II. MODEL

Details of the tight-binding quenched-molecular-dynamics method are given in an earlier paper.²² This formalism has been successfully used in the study of core structure of screw dislocation in hcp titanium²³ and for the multilayer reconstruction of W(100).²²

Here we give a brief outline of the calculation procedure. The relaxation is performed by integrating the equation of motion with the central difference algorithm.²⁴ We write

$$r_i(t + \Delta t) = 2r_i(t) - r_i(t - \Delta t) + \left[\frac{F_i(t)}{m} \right] \Delta t^2 + O(\Delta t^4), \quad (1)$$

$$v_i(t) = \frac{1}{2} \left[\left[\frac{r_i(t + \Delta t) - r_i(t - \Delta t)}{\Delta t} \right] \right] + O(\Delta t^3), \quad (2)$$

where $r_i(t)$, $v_i(t)$ are the position and velocity of the atom i at time t and $F_i(t)$ is the force acting on the atom i at this time.

The structure which minimizes the potential energy at 0 K is obtained within the quenching procedure, i.e., the velocity of an atom i is canceled when the product $F_i(t)v_i(t)$ is negative. The calculation of the force is done in the tight-binding formalism which we will now briefly summarize. The total energy of an atom i is written as

the sum of two contributions²⁵

$$E_i^{\text{coh}} = E_i^{\text{rep}} + E_i^{\text{band}}. \quad (3)$$

The first term E_i^{rep} is a pairwise repulsive potential of the Born-Mayer type:

$$E_i^{\text{rep}} = \sum_j A \exp(-pR_{ij}), \quad (4)$$

where R_{ij} is the bond length between atoms at sites i and j .

We limit the sum over j to first and second neighbors of atom i . The parameters A and p are determined so that the calculated equilibrium lattice constant and bulk modulus reproduce the experimental values (see Table I).

The second term E_i^{band} is the one-electron contribution due to d electrons. These d electrons are described by the following tight-binding Hamiltonian:

$$H = \sum_{\substack{i,j,\lambda,\mu \\ i \neq j}} |i,\lambda\rangle \beta_{ij}^{\lambda\mu} \langle j,\mu| + \sum_{i,\lambda} |i,\lambda\rangle \varepsilon_i \langle i,\lambda|, \quad (5)$$

where i and j are lattice sites, λ and μ are orbital labels ($\lambda, \mu = 1, \dots, 5$) and ε_i is the effective atomic energy level at site i . Taking this d atomic level as the origin of energies, $\varepsilon_i = 0$ for a bulk site: we neglect crystalline-field effects. The $\beta_{ij}^{\lambda\mu}$ are hopping integrals; using the simplest scheme they can be expressed in terms of three parameters only:²⁶ $dd\sigma$, $dd\pi$, and $dd\delta$. Moreover, any hopping integral $\beta(R)$ is a decreasing function of the interatomic distance R . A widely used phenomenological law is

$$\beta(R) = \beta(R_0) \left[\frac{R_0}{R} \right]^q. \quad (6)$$

The values for $dd\sigma$, $dd\pi$, $dd\delta$, and q are given by Masuda *et al.*²⁷ for Nb, Mo, and W and by Legrand *et al.*²² for Ta (see Table I).

The d -band energy may then be written as

$$E_i^{\text{band}} = \int^{E_F} E n_i(E, \varepsilon_i) dE - N_e \varepsilon_i, \quad (7)$$

where E_F is the Fermi level, $n_i(E, \varepsilon_i)$ the local density of states (LDOS) at site i , and N_e the d -band filling, which is given by the position of the Fermi level. ε_i is determined self-consistently at each step of the relaxation process by

assuming a local charge neutrality on each atom i :²²

$$\int^{E_F} n_i(E, \varepsilon_i) dE = N_e \quad \forall i. \quad (8)$$

ε_i is then different from zero for atoms near the surface and can be related to the experimental surface core level shift.²⁸

The LDOS is calculated using the familiar continued fraction expansion

$$n_{i,\lambda}(E, \varepsilon_i) = -\frac{1}{\pi} \lim_{\varepsilon \rightarrow 0^+} \text{Im} G_{ii}^{\lambda\lambda}(E + i\varepsilon), \quad (9)$$

with

$$G_{ii}^{\lambda\lambda}(z) = \langle i\lambda | \frac{1}{z - H} | i\lambda \rangle = \frac{1}{z - a_1 - \frac{b_1^2}{z - a_2 - \frac{b_2^2}{\ddots}}} \quad (10)$$

The coefficients a_n and b_n^2 (up to $n = 3$) are calculated using the recursion method and the usual square-root terminator.²⁹ As in Ref. 22, we take into account the energy variation up to the sixth neighbor to obtain the force with the needed accuracy. This is justified by the strong decrease of force constants in bcc transition metals beyond the sixth neighbor.³⁰ From a practical point of view, the calculation of the force on an atom i in one direction requires the knowledge of the energy variation on 65 atoms. Finally the relaxation is obtained with a good accuracy after 50 steps.

For the symmetrical surfaces (110), (100), and (111), we consider the perpendicular relaxations only, whereas for the unsymmetrical surfaces both perpendicular and parallel relaxations are allowed. The number of mobile layers increases for more open surfaces [from 6 for (110) to 12 for (210)].

III. RESULTS FOR THE SYMMETRICAL SURFACE

The relative relaxations of the first interlayer spacings are compared in Table II to the corresponding experimental values for the three symmetrical surfaces of Nb, Ta, Mo, and W. As pointed in Ref. 1, the top-layer relaxation increases with the increasing roughness at least for

TABLE I. Values of the parameters N_e , A , q , and pR_1^0 (where R_1^0 is the equilibrium distance between first neighbors), $dd\sigma$, $dd\pi$, $dd\delta$, and of the resulting cohesive energies.

	Nb	Ta	Mo	W
N_e	3.7	3.3	4.4	4.4
A (eV)	4094	8726	11 410	18 122
q	3.32	3.0	3.57	3.26
pR_1^0	9.26	10.23	10.23	10.65
$dd\sigma$ (eV)	-1.12	-1.37	-1.17	-1.22
$dd\pi$ (eV)	+0.87	+0.75	+0.88	+1.04
$dd\delta$ (eV)	-0.35	0	-0.33	-0.50
E^{coh} (eV/atom)				
Calc.	-7.0	-7.3	-7.4	-9.0
Expt.	-7.5	-8.0	-6.7	-8.7

TABLE II. Relative variation of the first interlayer spacing $\Delta d_{12}/d$ (%) for the three symmetrical surfaces; d is the bulk interlayer distance.

	(110)	(100)	(111)
Nb	-3.6	-6.3	-21.5
Ta	-3.8	-6.3	-21.6
		expt. -11 ^a	
Mo	-3.3	-6.9	-19.7
	expt. -1.6 ^b	expt. -9 ^c	
W	-1.4	-3.5	-16.3
	expt. < 2 ^d	expt. -3 to -10 ^e	

^aFrom Ref. 33.

^bFrom Ref. 34.

^cFrom Ref. 36.

^dFrom Refs. 52 and 43.

^eFrom Refs. 53 and 39.

symmetrical surfaces. The agreement with experiments is rather good considering the experimental uncertainties [for instance experimental $\Delta d_{12}/d$ is between -3% and -10% for the most studied surface, W(100)], and the parameter dependence of the model. For different realistic values of the hopping integrals³¹ and d -band filling, we obtain the following variations for $\Delta d_{12}/d$: for Ta(100), -6.3 to -9.8; for Ta(111), -21.6 to -27.8; for W(100), -3.5 to -4.3; and for W(111), -16.3 to -19.1.

More interesting is the relaxation profile (Table III). For the close-packed faces (110) and (100) we find that the relaxation is principally confined to the first plane, with small deviations for Ta(100). This is in good agree-

ment with experiments³²⁻³⁶ and other calculations.^{18,37} For the (111) face, we obtain a "contraction, contraction, expansion, contraction" sequence for d_{12} , d_{23} , d_{34} , and d_{45} in all metals. This is the sequence obtained experimentally on Fe,³⁸ and it seems roughly metal-independent, at least for bcc transition metals.

All the results presented here are obtained for the unreconstructed surfaces, i.e., we allow only rigid translation of the surface layers. However, it is well known that W(100) and Mo(100) are reconstructed at low temperature.³⁹

The same model has been successfully used to predict the multilayer reconstruction of W(100).²² Concerning the stability of W(110), some experiments⁴⁰ have suggested that the surface atoms occupy the threefold coordinated positions (and not the twofold ones as in the normal lattice site), i.e., the surface is rigidly translated along the $\langle 110 \rangle$ direction. A tight-binding calculation⁴¹ performed with one mobile layer predicts that the unreconstructed surface is the most stable. We obtain the same result here with six mobile layers. Starting from the reconstructed geometry, the system goes spontaneously towards the unreconstructed position. It is a good example of the independence of the equilibrium configuration from the initial one, as already mentioned.²² The stability of the unreconstructed W(110) face is in agreement with LEED experiments.^{42,43}

IV. RESULTS FOR THE UNSYMMETRICAL SURFACES

If the surface is unsymmetrical, the relaxation can have parallel as well as perpendicular components. It is the case for the (211), (310), and (210) bcc surfaces. Experiments on these surfaces are up to now very scarce and, to our knowledge, only a systematic study of iron surfaces³⁻⁵ and LEED results on W(211) (Ref. 44) are available.

In Table IV we present the values of the first-layer relaxation. Δa_{ij} is the parallel shift of the i th layer with respect to the j th layer, and a is the spacing along the closer-packed rows for (211), and perpendicular to the closer-packed rows for (210) and (310). By convention, the sign of Δa is positive when the top layer shifts so that

TABLE III. Profile of the multilayer relaxation for the three symmetrical surfaces. Δd_{ij} is the change in the perpendicular distance between the i th and j th layers.

	ij	$\Delta d_{ij}/d$ (%)		
		(110)	(100)	(111)
Nb	12	-3.6	-6.3	-21.5
	23	-0.5	-0.7	-11.4
	34			+7.5
	45			-0.8
Ta	12	-3.8	-6.3	-21.6
	23	+1.0	-1.9	-8.6
	34	-0.5	+1.9	+11.8
	45		-0.4	-3.9
	56			+0.2
Mo	12	-3.3	-6.9	-19.7
	23	-0.7	-1.1	-7.6
	34			+3.8
	45			-2.5
	56			-1.6
	67			-0.4
W	12	-1.4	-3.5	-16.3
	23	-0.4	-0.6	-7.8
	34			+7.3
	45			-1.1
	56			-1.9
	67			0

TABLE IV. Values of the relative perpendicular $\Delta d_{12}/d$ and parallel $\Delta a_{12}/a$ relaxation of the first layer for the three unsymmetrical surfaces (%). See the text for the sign convention concerning $\Delta a_{12}/a$.

	(211)		(310)		(210)	
	$\Delta d_{12}/d$	$\Delta a_{12}/a$	$\Delta d_{12}/d$	$\Delta a_{12}/a$	$\Delta d_{12}/d$	$\Delta a_{12}/a$
Nb	-15.5	+4.9	-23.7	-7.4	-23.7	-4.9
Ta	-9.2	+2.9	-14.9	-3.0	-19.0	-3.1
Mo	-13.9	+4	-20.0	-8.0	-22.4	-6.0
W	-10.8	+6.0				
Expt. ^a	-12.4	+9.0				

^aFrom Ref. 44.

second-layer atoms get closer to the center of first-layer meshes (this convention is not the same as in JJM). Table IV shows two important points: (i) Despite the fact that the roughness of the (310) face (as defined in Ref. 1) is smaller than that of the (111) face, the contraction of the first layer is slightly more important for the unsymmetrical surface, except for Ta. This behavior is indeed observed in Fe, and obtained in JJM. (ii) The direction of the parallel displacement depends on the crystallographic orientation of the surface. For the (211) surface, the parallel shift is always towards a higher symmetry of the first layer with respect to the second layer. This is in agreement with experimental results on W(211) and Fe(211), and with the calculation of JJM. Note that the second moment approach of the tight-binding scheme

with hopping integrals between nearest neighbors only gives the wrong sign for the parallel displacement of W(211).⁴⁵

In contrast, for the (310) and (210) surfaces we obtain a displacement towards the less symmetrical position of the first layer relative to the second layer (negative sign of Δa_{12}), contrary to what is observed experimentally for Fe. Note, however, that a negative sign of Δa_{12} has been put in evidence for Ni(311).⁴⁶ From the theoretical point of view JJM find a negative Δa_{12} (with our convention) for Fe(210) and a positive Δa_{12} for Fe(310). In fact, it seems that parallel displacements are more difficult to obtain, both experimentally and theoretically, one reason being perhaps that the first-layer shift is not necessarily the most important.^{15,46}

TABLE V. Profile of the multilayer relaxation for the three unsymmetrical surfaces. $\Delta d_{ij}/d$ ($\Delta a_{ij}/a$) is the relative perpendicular (parallel) relaxation between the i th and j th layers (%). See the text for the sign convention concerning $\Delta a_{ij}/a$.

	ij	(211)		(310)		(210)	
		$\Delta d_{ij}/d$	$\Delta a_{ij}/a$	$\Delta d_{ij}/d$	$\Delta a_{ij}/a$	$\Delta d_{ij}/d$	$\Delta a_{ij}/a$
Nb	12	-15.5	+4.9	-23.7	-7.4	-23.7	-4.9
	23	+2.4	+2.9	+5.9	+5.2	-9.6	-2.4
	34	-1.5	+0.1	-1.0	-0.6	+6.3	+4.3
	45			-2.7	+0.4	+1.6	0
	56			-0.2		-10.5	
	67					+3.2	
	78					+1.5	
Ta	12	-9.2	+2.9	-14.9	-3.0	-19.0	-3.1
	23	-0.8	-1.9	+0.8	+2.1	-0.5	-0.8
	34	+1.3	+0.9	-3.0	-0.4	-1.2	+2.1
	45	-0.4		+1.2	+0.6	-5.4	0
	56			+0.4		+0.8	
Mo	12	-13.9	+0.4	-20.0	-8.0	-22.4	-6.0
	23	+1.9	+5.1	+3.0	+3.4	-4.1	-2.5
	34	-2.4	-0.9	+0.3	-0.6	+0.4	+3.2
	45	-0.9	+0.3	-3.5	+0.3	+3.3	0
	56			+0.3		-8.1	
	67					-0.4	
W	12	-10.8	+6.0	-16.9	-3.3	-19.9	-2.7
	23	+3.3	-1.6	+5.2	+1.4	-5.0	-0.9
	34	-1.2	+0.3	-1.2	+0.2	+7.7	+1.4
	45	-0.5		-1.0		-1.3	0.4
	56			+0.1		-5.8	
	67					+2.4	
					0.7		

TABLE VI. Shear elastic constants C_{44} and C' in eV atom⁻¹, calculated within the seventh-moment approximation (noted μ_7) and the nineteenth-moment approximation (noted μ_{19}). Experimental values are from Ref. 51.

	C_{44}			C'		
	μ_7	μ_{19}	Expt.	μ_7	μ_{19}	Expt.
Nb	4.2	2.5	3.2	3.9	4.4	6.3
Ta	12.2	11.5	9.2	8.1	5.0	5.8
Mo	6.1	9.1	10.6	9.1	11.2	13.7
W	12.1	14.0	15.7	8.9	11.3	15.7

In Table V we show the in-depth behavior for the unsymmetrical surfaces. We note that the profile of the perpendicular relaxations is once more again roughly universal with small deviations for Ta; it is a succession of “contraction, dilatation, contraction” for (211) and (310) and “contraction, contraction, dilatation” for (210). These results are in excellent agreement with the experimental ones obtained for Fe.³⁻⁵

Concerning the profile of the parallel displacements, the situation is not so simple. For the (310) and (210) surfaces, we obtain the same behavior for the four studied metals, with the following oscillatory pattern of signs: $-+$ for (310) and $--+$ for (210). This is different from experimental results on Fe, which are $++$ for (310) and $+++$ for (210). Moreover, JJM find in their empirical approach other signs: $+-$ for (310) and $-++$ for (210). For the (211) surface, the profile of the parallel shift is metal dependent, but there is no experimental result to confirm this prediction.

V. COMPARISON WITH OTHER THEORETICAL WORK AND DISCUSSION

As noted in the introduction, JJM have studied the same surfaces that we have. Their work is based on the use of an empirical electrostatic model, with one fitting parameter, which stiffens the force constant that tries to restore the ions to their bulk positions. This parameter is determined by fitting to experiments the calculated relaxations for Fe. (In fact, the parameter is not strongly metal dependent; it is the same for Fe and Al, and is not very different for Cu.^{14,15}) In comparison, in our semi-empirical tight-binding model, all parameters are fitted to bulk properties and differ from one metal to another (number of d electrons, bulk modulus, . . .), which allows us to predict some metal-dependent properties for the relaxation profile.

When we compare our results with those of JJM, we see that the perpendicular relaxations are roughly similar both for the magnitude and the profile. It is not the case for the parallel shifts, which are more sensitive to the model of the total energy, and which are not metal-independent, at least for the (211) face.

In fact, the difficulty to predict the correct parallel displacement is not new; we have already pointed out the

wrong sign in the second moment study of W(211).⁴⁵ There is the same failure for the parallel displacement of the second layer of the reconstructed (110) face of Pt and Au.⁴⁷⁻⁴⁹

In the present study we have observed important variations (even the sign can change for the parallel relaxations) when we use other parameters,³¹ which give a more serious disagreement for the elastic constants. We present in Table VI the values of the calculated elastic constants with our seventh-moment approximation and with the nineteenth-moment approximation (which is better but too time consuming for the calculation of the multilayer relaxation). We see that the agreement is not perfect and this has to be related to the study of Allan and Lannoo.³⁷ Actually, these authors have shown that the asymptotic behavior of the relaxation is given by the bulk-phonon dispersion relations in the complex plane. Even though their approach is valid only for the asymptotic behavior (whereas we are mainly concerned here with the movement of the first layers), it shows that the model used to study surface relaxations must predict bulk-phonon dispersion relations. From this point of view, it is encouraging to see that the tight-binding model reproduces all the observed anomalous structure of the phonon dispersion in bcc transition metals^{30,50} and it would be very interesting to check the corresponding ability of the model of JJM.

VI. CONCLUSION

We have presented a tight-binding study of the multilayer relaxation in bcc transition metals. Compared to the only systematic experimental analysis on Fe, our model gives correct results for the magnitude and the profile of the perpendicular relaxations, which are roughly metal independent. For the parallel relaxations, we suggest that the profile can change from one metal to another. To check this suggestion, it would be highly desirable to perform experimental studies on open surfaces of other bcc transition metals.

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