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Nonempirical potentials in modelling of boron adhesion on a (110) tungsten surface

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Abstract

We have performed the atomistic simulations of the adhesion process of a boron atom on a tungsten(110) surface on the basis of the generalized simulation annealing formalism. The interatomic potentials used in these simulations were obtained from *ab initio* total energy calculations on the basis of the recursion procedure. The nonempirical calculations have been carried out in the framework of density functional theory in the coherent potential approximation.

(Some figures in this article are in colour only in the electronic version)

1. Introduction

Systems in which a metalloid is deposited on a metal continue to grow in importance and in the variety of their applications [1, 2]. In exploitation, whether as catalysts, in recording media, in metal–matrix composites or in various microelectronic devices, the adsorption of the metalloid atoms on a metallic substrate is often crucial. Nevertheless, due to the complexity of these systems the important details of the metalloid–substrate interactions are still unclear. The microscopic features of metal–metalloid interfaces including the reconstruction of the surface where the metalloid atom is adsorbed are only rarely known from direct measurements [3].

Yet there remain widely varying views on the nature of the metal–metalloid interfacial bonding and on the microscopic mechanism of metalloid adsorption or film growth. Despite much theoretical work on the adhesion of metal or metalloid atoms on regular metal substrates, using widely varying models and computational methods, there is still a lack of full understanding of the adhesion process and of properties of the adatom–substrate system on the atomic scale. Partly this is caused by the existence of the sensitive balance of contributions to the energy of a metalloid atom on a metal substrate. Some aspects of adsorption of O, H and C on low-index W surfaces were studied recently [4] showing the importance of both chemical

and structural effects in the binding of adsorbed atoms to the surface. In this communication we demonstrate that interatomic potentials [5] that we use in our simulations allow us to obtain fine features in adsorption of a boron atom on the tungsten(110) surface. The advantage of the developed potential is straightforward—actually it does not contain adjustable parameters to obtain better agreement with experiments and is absolutely *ab initio*.

We illustrate directly the importance of directional bonding in simulations of the adsorption process on the tungsten(110) surface. The tests of the many-body potential for tungsten have proved its high quality to reproduce properties where relaxation is of crucial importance.

2. Methodology

2.1. Nonempirical many-body potentials

According to [6] the nonempirically calculated dependence of the cohesive energy, E , on the distance in the case of pairwise interactions could be written in the form

$$E(r) = \sum_{p=1}^{\infty} n_p V(s_p r), \quad (1)$$

with the atomic separation grouped into coordination shells p of radius $s_p r$, containing n_p atoms each. Uniform dilatation of the lattice is described by varying the parameter r with the structural quantities $\{s_p\}$ and $\{n_p\}$ fixed. The shells are numbered so that $s_1 < s_2 < s_3 < \dots$, and the distances scaled so that $s_1 = 1$. The recursive substitution generates now the explicit formula

$$V(r) = \frac{1}{n_1} E(r) - \sum_{p=2}^{\infty} \frac{n_p}{n_1^2} E(s_p r) + \sum_{p,q}^{\infty} \frac{n_p n_q}{n_1^3} E(s_q s_p r) - \dots \quad (2)$$

This way the *ab initio* effective pair potentials for tungsten and boron were obtained (for details see [5]).

We study the many-body interactions with the scheme of [6] that considers the simplest case of a many-body potential with volume-independent pair terms and separable three-body terms. Subtracting the pair terms from the *ab initio* calculated $E(r)$ forms the many-body energy term, $F(r)$

$$F(r) = E(r) - E^{(pair)}(r), \quad (3)$$

where $E^{(pair)}(r)$ is the energy that is presented as a sum over pairwise interactions. The function $F(r)$ is expressed as a sum over pairs of bonds

$$F(r) = \sum_i \sum_{\substack{j \neq i \\ j > i}} \sum_{\substack{k \neq i, \\ k > j}} g(r_{ij}) g(r_{jk}) h(\vartheta_{ijk}), \quad (4)$$

with $\cos \vartheta_{ijk} = (\vec{r}_{ij} \vec{r}_{jk}) / (r_{ij} r_{jk})$ and $r_{ij} = |\vec{r}_i - \vec{r}_j|$. We use $h(\vartheta_{ijk})$ in the same form as in [6]. According to [6–8] $F(r) \geq 0$. It may be shown that accounting for three-body interactions is equivalent to the representation of the energy in terms of effective interactions, $\Phi(\vec{r}_i, \vec{r}_j)$ by $E(r) = \frac{1}{2} \sum_{\substack{i,j \\ i \neq j}} \Phi(\vec{r}_i, \vec{r}_j)$, where

$$\Phi(\vec{r}_i, \vec{r}_j) = V(|\vec{r}_i - \vec{r}_j|) + \sum_{k, k \neq i, k > j} g(|\vec{r}_i - \vec{r}_j|) \times g(|\vec{r}_j - \vec{r}_k|) \times h(\vartheta_{ijk}). \quad (5)$$

Here the first term is the pairwise potential and the second one describes the triple interaction as the angular dependent interaction of two bonds. These bonds are given by the vectors \vec{r}_{ij} and \vec{r}_{jk} .

Development of the interatomic potential for tungsten and boron atoms has been started from the nonempirical total energy calculations for the binary disordered alloy and its components. The total energies have been used to define the mixing energy, ΔE , as a function of the lattice parameter

$$\Delta E = E_{\text{alloy}} - [cE_{\text{B}} + (1 - c)E_{\text{W}}], \quad (6)$$

where c is the atomic fraction of boron and E_{B} and E_{W} are the energies of the components. In the regular solid solution model approximation the mixing energy can be written in terms of the constant of interaction U that also depends on the lattice parameter.

$$\Delta E = Uc(1 - c). \quad (7)$$

According to [9, 10] this constant may be defined in terms of interatomic W–W, B–B and W–B interactions, and we can write the sum of W–B interatomic potentials in the form

$$\delta E = \sum_{\substack{i,j \\ i \neq j}} V_{\text{WB}}(|\vec{r}_i - \vec{r}_j|) = U + E_{\text{W}} + E_{\text{B}}. \quad (8)$$

This result solves the problem of determination the tungsten–boron interatomic potential because equation (8) may be rewritten in the same form as equation (1). After that the recursion scheme given by equations (2)–(5) may be applied. For details we refer to our recent paper [5]. The effective interatomic potential $V_{\text{WB}}(r)$ may be calculated with the recursion formula (2), with the substitution $\delta E(r)/2$ for $E(r)$.

2.2. Atomistic simulations

In atomistic simulations we used the MC methodology in the generalized simulated annealing approach (GSA) (see, for example, [11] and references therein). GSA is based on the correlation between the minimization of a cost function (conformational energy) and the geometry randomly obtained through slow cooling. In this technique, an artificial temperature is introduced, and the system is gradually cooled in a complete analogy with the annealing technique used in metallurgy when a molten metal reaches its crystalline state (the global minimum of the thermodynamic energy). In our case the temperature plays the role of an external noise. Simulated annealing methods have been applied successfully due to their suitability for large-scale optimization problems, especially for those in which a desired global minimum is hidden among many local minima. The basic aspect of the simulated annealing method is that it is analogous to thermodynamics, especially concerning the way that liquids freeze and crystallize, or that metals cool and anneal. At high temperatures, the atoms move freely with respect to one another. If the system is cooled slowly, thermal mobility is lost. The atoms, say in complicated molecules, are often able to line themselves up and assume a molecular geometry that is in general a local equilibrium state. The simulated annealing procedure is actually more complicated than the combinatory one, since the known problem of long, narrow potential valleys asserts itself. Simulated annealing tries random steps, but in a long, narrow valley almost all random steps are uphill. The amazing fact is that for a slowly cooled system, nature is able to find this minimum energy state. So the essence of the process is slow cooling, allowing sample time for redistribution of the atoms as they lose their mobility. This is the technical definition of annealing, and it is essential for ensuring that the lowest energy state will be achieved.

The artificial temperature (or a set of temperatures) acts as a convenient stochastic source for eventual detraining from local minima. The procedure of searching the minima (global and local) or mapping the energy hypersurface consists of comparing the energies of two

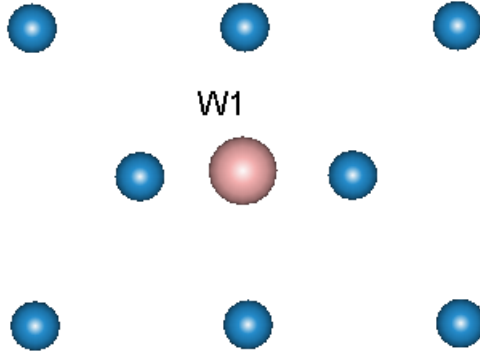


Figure 1. A top view on the tungsten (110) surface. W1 marks the position of simulated adsorption of a boron atom at the surface.

consecutive random geometries x_{t+1} and x_t obtained from the GSA routine. Here x_t is a N -dimensional vector that contains all atomic coordinates (N) to be optimized. For details of our MC approach see [12, 13].

2.3. Structural optimization

We simulated the adhesion process of a boron atom on the tungsten(110) surface and studied a site occupation preference for the boron atom. The surface was simulated in a cluster approximation with 393 atoms. In figure 1 we show the site selected for our simulations of the adsorption process. This site is the centre of the rhomboid (site W1). The primary task in our search for well converged statistical averages for the geometry relaxation process in the model cluster was the selection of the number of GSA loops. In our GSA simulations we used the GSA in the standard formulation [11]. The maximum atomic displacement was adjusted to the lattice parameter, a , to ensure its acceptance ratio to a did not exceed 0.5. We are able to conclude on the basis of this analysis that a good convergence could be achieved for a number of GSA loops not less than 10^6 .

3. Results and discussion

3.1. Nonempirical calculations and development of interatomic potentials

3.1.1. Tungsten interatomic potential. The total energy calculations have been performed in the scalar-relativistic approach for a number of different volumes per atom. Core electrons were frozen after initial atomic calculations. All the calculations were fulfilled in the framework of the LMTO method [14]. The convergence criterion for the total energy was equal to 0.001 mRyd. Typically 60 iterations were needed to achieve the necessary convergence. The equilibrium lattice parameter a for tungsten is 3.244 Å from our nonempirical calculations ($a_{exp} = 3.165$ Å from [15]). We have calculated the tungsten cohesion energy, E , as a function of a . It gives $E = -0.632$ Ryd/atom for the equilibrium a , which is in good agreement with experiment (-0.637 Ryd/atom [16]). The dependence $E(a)$ was used to calculate the pairwise potential $V(r)$ by means of the recursion formula, as discussed above. To avoid the convergence problem in *ab initio* calculations of a strongly expanded lattice the smooth approximation for the tail of $E(a)$ was used. $V(r)$ is well represented by the Morse-type function

$$V(|\vec{r}_i - \vec{r}_j|) = D[e^{-2\lambda(|\vec{r}_i - \vec{r}_j| - r_0)} - 2e^{-\lambda(|\vec{r}_i - \vec{r}_j| - r_0)}] \quad (9)$$

where $D = 0.04775$ Ryd, $\lambda = 0.8233$ au⁻¹ and $r_0 = 5.15278$ au. We found that the averaged relative difference in $V(r)$ is less than 0.1% while changing the cut-off radius from the seventh to the eighth shell. To examine the quality of the obtained potential and the validity of the procedure used, the Debye temperature for W was calculated using the same methodology as in [17]. The obtained value, 410 K, is in excellent agreement with the measured 392 K. The boron interatomic potential was obtained in the same manner.

The procedure described above was used to obtain the radial distribution function $g(r)$. After numerical calculation with equations (3) and (4), $g(r)$ was approximated by the polynomial function

$$g(r) = \begin{cases} \sum_{i=0}^9 A_i r^i, & \text{if } 1.3 \text{ au} \leq r \leq 5.85 \text{ au} \\ 0, & \text{if } r > 5.85 \text{ au.} \end{cases} \quad (10)$$

The coefficients A_i for W are $A_0 = -15.619116$, $A_1 = 45.701973$, $A_2 = -54.436842$, $A_3 = 36.649062$, $A_4 = -15.482778$, $A_5 = 4.264667$, $A_6 = -0.767412$, $A_7 = 8.71983 \times 10^{-2}$, $A_8 = -5.690853 \times 10^{-3}$ and $A_9 = 1.628766 \times 10^{-4}$. This gives the value of $g(r)$ in (Ryd)^{1/2} for the distances measured in au.

We checked the applicability of this tungsten interatomic potential to some properties where the relaxation effects are important and play a substantial role. The GSA approach was used for calculations of relaxation. The energy of the vacancy formation obtained in our simulations is $E_f^{(v)} = 4.23$ eV. This is in good agreement with experimental data [18] and the results of other calculations. We have also calculated the value of the diffusion barrier for the self-diffusion in W by simulating the movement of the atom from the position $(a/2)(111)$ to $(a/2)(000)$ where the vacancy was situated. We have relaxed the lattice at each step of this process. The obtained migration energy for the self-diffusion in W is equal to 1.67 eV. This result is also in good agreement with the measurements (1.63 eV from [18, 19]).

3.1.2. Calculation of interatomic potential for tungsten–boron interactions. Herewith we will briefly explain the scheme of our calculations of the interatomic potential for tungsten–boron interactions (for details see [5]). Using the LMTO method in the framework of the coherent potential approximation (CPA) (for details of CPA LMTO calculations see [20, 21]) we have calculated the total energies of the W–B alloy with the boron concentration equal to 5 at.% for different lattice parameters. These energies were used to determine the mixing energy according to equation (6). The partial energies for the tungsten and boron constituents, E_B and E_W , of the alloy have been calculated in the same bcc lattice in the framework of the LMTO formalism. The constant of interaction U for a number of lattice parameters $\{a_i\}$ was calculated according to equation (7), and (8) was used for the calculations of the dependence of δE on a . After the substitution of $\delta E(r)/2$ for $E(r)$ in equation (2) we have applied the recursion procedure to calculate the nonempirical W–B interaction potential, $V_{WB}(r)$.

3.2. Simulations of the boron adhesion process

The many-body interatomic potential $\Phi(r)$ and the nonempirical W–B interaction potential $V_{WB}(r)$ were applied to simulate the adhesion process of a boron atom on a tungsten(110) surface in the centre of the rhomboid (see figure 1). We have placed a trial boron atom in a number of positions selected on the path perpendicular to the surface (110) (figure 2). For each of these positions we found an equilibrium spatial structure of the cluster with the boron atom in the trial position. Thus the adhesion process that is simulated in our study is a very slow (compared to the characteristic time of the lattice relaxation) movement of the boron

Table 1. Calculated displacements of tungsten atoms during the boron adsorption process. Numbers of corresponding atoms are given in figure 3(a).

| Marked tungsten atoms | | Displacements of tungsten atoms (Å) (Distance of boron atom to the (110) surface) | | | | | | Displacements of tungsten atoms, (% of the interlayer distance) (Distance of boron atom to the (110) surface) | | | | | |
|-----------------------|---|--|-------|-------|-------|-------|-------|--|------|------|-------|------|------|
| | | 0 Å | 1 Å | 3 Å | 3.5 Å | 4 Å | 6 Å | 0 Å | 1 Å | 3 Å | 3.5 Å | 4 Å | 6 Å |
| 1st layer | 1 | 0.567 | 0.679 | 1.083 | 0.963 | 0.861 | 0.647 | 24.7 | 29.6 | 47.2 | 42.0 | 37.6 | 28.2 |
| | 2 | 0.934 | 0.807 | 0.306 | 0.458 | 0.910 | 0.920 | 40.7 | 35.2 | 13.3 | 20.0 | 40.0 | 40.0 |
| | 3 | 0.401 | 0.198 | 0.629 | 0.702 | 0.162 | 0.268 | 17.5 | 8.7 | 27.4 | 30.6 | 7.0 | 11.7 |
| | 4 | 1.031 | 0.162 | 0.652 | 0.773 | 0.282 | 0.188 | 45.0 | 7.1 | 28.4 | 33.7 | 12.3 | 8.2 |
| | 5 | 0.290 | 0.420 | 0.323 | 0.362 | 0.420 | 0.418 | 12.6 | 18.3 | 14.1 | 15.8 | 18.3 | 18.2 |
| 2nd layer | 6 | 0.169 | 0.943 | 0.835 | 0.914 | 0.942 | 0.954 | 7.4 | 41.1 | 36.4 | 39.8 | 41.1 | 41.1 |
| | 7 | 0.281 | 0.216 | 0.275 | 0.282 | 0.207 | 0.089 | 12.2 | 9.4 | 12.0 | 12.3 | 9.0 | 3.9 |
| 3rd layer | 8 | 0.266 | 0.283 | 0.257 | 0.271 | 0.282 | 0.281 | 11.6 | 12.3 | 11.2 | 11.8 | 12.3 | 12.3 |

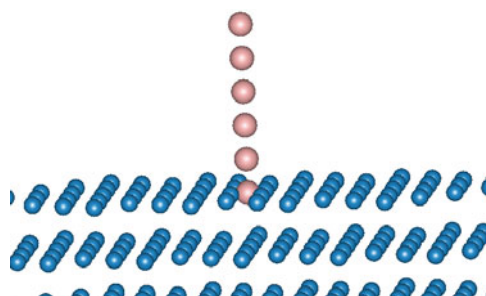


Figure 2. A side view of the tungsten cluster with (110)-terminated surface and different positions of the boron atom that present the simulated adsorption path.

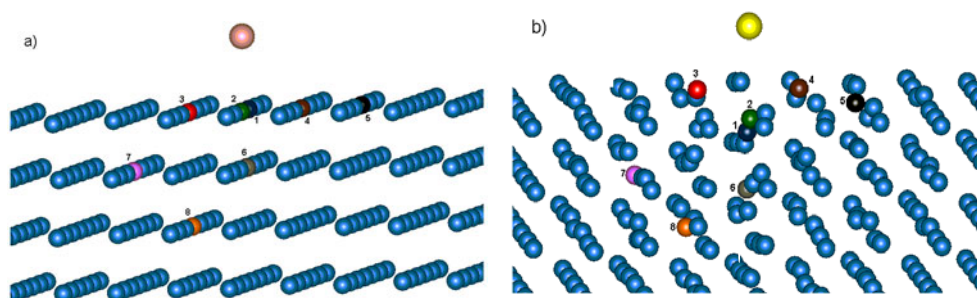


Figure 3. Relaxed and nonrelaxed tungsten clusters with the boron atom at a distance of 3 Å above the surface.

atom to the surface. The cluster was relaxed using the GSA procedure for 10^6 GSA loops. The GSA procedure was used to simulate the relaxation. The convergence of the relaxation process was achieved after approximately 10^6 GSA loops for each position of the boron atom. As an example the final structure of the selected cluster with the boron atom 3 Å from the surface is shown in figure 3. In figure 3(a) we select some atoms in different layers in the vicinity of the surface to observe their relaxation for a number of the boron atom positions on the simulated adhesion path. In figure 3(b) the final structure of the cluster with the boron atom at the distance 3 Å from the surface is shown. Displacements of the atoms selected in figure 3 for different trial distances of the boron atom are presented in table 1. The results of calculations of the energy of the system for the adhesion path of the boron atom are plotted in figure 4. In this figure the change in the energy with respect to the energy of the tungsten cluster with a (110) surface and the boron atom placed at a distance equal to 6 Å from the surface is demonstrated. The same procedure was carried out in the pairwise approximation (the dashed curve in figure 4) and with the three-body interactions (the solid curve). Figure 4 shows that the pairwise interaction overestimates the value of the adsorption barrier and that the three-body potential is responsible for the shift of the adsorption barrier outward from the cluster. The position of the energy minimum is situated at a distance equal to 1 Å above the surface.

At the same time, accounting for the many-body interactions changes sufficiently the local reconstruction of the lattice in the vicinity of the surface. It is obvious from figure 4 that the adhesion process starts from a distance approximately equal to 5 Å. The displacements of atoms presented in table 1 for the boron at a distance of 6 Å from the surface may be considered as corresponding to the case of the ‘pure’ (110) surface of tungsten. It is interesting to note

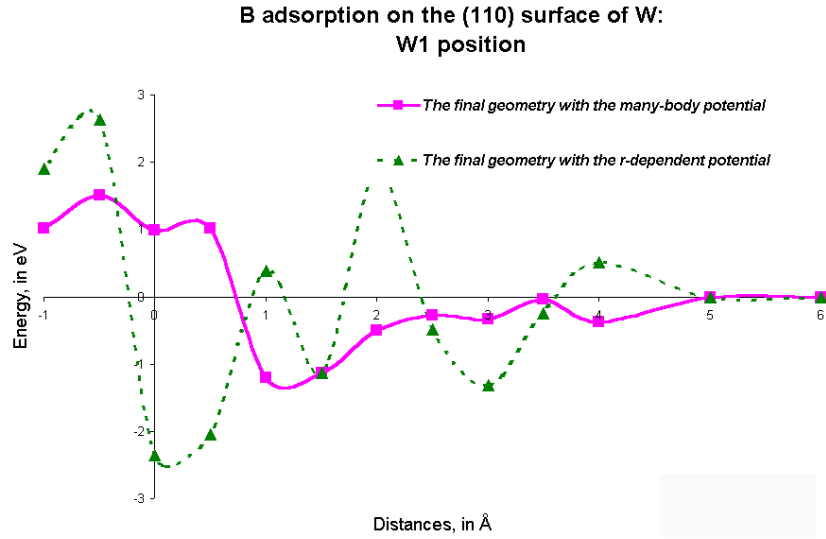


Figure 4. The energy profile along the path in the simulated adsorption process. See explanatory remarks in the text.

that the values of displacements of tungsten atoms in the vicinity of the (110) surface when the boron atom is moving to the surface along the adsorption path are often lower than those for the ‘pure’ surface. This indicates the existence of a complicated balance between W–B and W–W interactions in the adsorption process.

Several additional comments should be given to clarify the results obtained in our approach in the study of B adsorption on a W(110) surface. The first one concerns the application of the adiabatic hypothesis used in our simulations where the boron atom slowly moves to the surface of tungsten. It is easy to estimate that the mean-square velocity $\sqrt{v_z^2}$ at room temperature for a boron atom that moves to a tungsten surface in the z -direction (as schematically shown in figure 2) is close to 500 m s^{-1} . In the case of chemical vapour deposition in the inert gas atmosphere the mass transfer of the B atoms occurs with drift velocities at least one order smaller as compared with $\sqrt{v_z^2}$. The velocity of sound in W has the order of magnitude 10^3 m s^{-1} . Thus, for such a type of process as vapour deposition, relaxations of the atoms in the vicinity of the W surface in our simulations that include $\sim 10^6$ loops are complete at each distance of B from this surface. Obviously it would be of interest to use MD simulations to study the case when the velocity of the B atom that approaches the surface is high: how this atom is stopped by the repulsion interaction and what the changes in surface relaxations are in comparison with the so called slow movement of the adsorbed atom.

W–B interaction forces are rather short ranged. The distance of 5 \AA (see figure 4) when the approaching B atom starts to ‘feel’ the W(110) surface is only $\sim 15\%$ larger than the interplanar distance in W in the direction (110). As yielded by [5] actually the pairwise part of the W–B interaction is much more short ranged in comparison with the W–W interatomic interaction. According to our calculations even the very fast decreasing part of W–B interaction nevertheless has a small tail. The origin of this tail is that this interaction is obtained from the recursive procedure for B interstitials in the bulk tungsten. The potentials used in our calculations include both pairwise and three-body angle-dependent interactions. By the definition these three-body terms in the energy are not additive.

The damping of oscillations by three-body interactions (see figure 4) is an expected result. At small distances we observe the pronounced angle-dependent interaction that makes the lattice more stable with respect to the atomic displacements. This result qualitatively corresponds to the numerous papers describing the stabilizing of the lattice by many-body interactions in a phonon spectrum. Keeping this fact in mind, the smoothening of the curve is the relevant result that shows simply that the pairwise approximation overestimates the elastic response of the W surface to the excitation that comes from the B atom that approaches the surface. It is worthwhile to mention that oscillations of the energy in figure 4 are not related to Friedel oscillations. On one hand it is not the result of the self-consistent screening in the electron gas. On the other hand these oscillations are not so surprising while recalling the oscillations of the deformational interaction in substitutional or interstitial (even more) solid solutions. In this case we simply deal with the waves of the matrix atom displacements. These waves of displacements correspond to the oscillating interactions of the impurity with the matrix atoms. Such a result is well known in phenomenological microscopic elastic theory (see, for example, [22]). One of the internal parameters in the GSA approach is the radius of some effective sphere surrounding each atom. The treatment of the possible atomic positions for each atom (to find the equilibrium structure) is thus limited by the corresponding volume. The atomic displacements are not allowed to overcome these limits. So, the oscillations that we see in figure 4 may be associated indirectly with some type of cut-off effect in the phonon dispersion. At the same time the chosen radius is large enough to escape the influence of this cut-off effect at least for the case of not extremely high temperatures. Finally, let us discuss the nature and interpretation of the adhesion process illustrated by figure 4. The smallest energy minimum in figure 4 is situated at the distance 4 Å that is a little bit smaller than the interplanar distance 4.2 Å in the direction normal to the surface (110) in W. This result together with the depth of this minimum, that is approximately 0.35 eV (compare for Ag on MgO, where Ag occupies positions above oxygen and the adsorption energy is about 0.25 eV [23]), seems to be reasonable. The order of magnitude is the same in these quite different cases. The analysis of W atom displacements shows that at distances more than 4 Å the boron atom does not influence the reconstruction of the W surface. This allows us to conclude that the formation of the minimum of the energy curve from figure 4 at this distance is the result of the interaction of the B atom with the already relaxed W(110) surface. This means that even if the B atom moves to the surface with a high velocity it will feel the field of this relaxed surface. At smaller distances to the surface B influences the relaxation of W atoms at the surface. If B still has kinetic energy to overcome the potential barrier in the vicinity of 3.5 Å it will interact with the W(110) surface, and this interaction will lead to the additional relaxation of the tungsten atoms in the vicinity of the surface stimulated by boron. The boron atom will lose most of its kinetic energy and will start to move slowly towards the surface. The energy profile of its interaction with the surface is displayed in figure 4 for distances less than 3.5 Å and accounts for the additional relaxation of W(110) surface stimulated by this interaction. The B atom will be stopped at a distance approximately equal to 1 Å at a very deep energy minimum.

When the B atom moves slowly to the W(110) surface it will be localized in a small minimum, i.e. its adsorption will occur at a distance of about 4 Å from the surface. The small value of this adsorption energy allows us to assume that in these conditions we will have the case of physisorption. Of course, if the kinetic energy of the B atom is higher than the absolute value of the adsorption energy, this atom will not be stopped at the distance corresponding to this minimum. It will continue to move until it is captured in the deeper minimum that is much closer to the surface. The velocity of the B atom movement will be sufficiently decreased because it loses its kinetic energy by interaction with the relaxed W surface at a distance of ~ 4 Å. The velocity of the further movement towards the surface is relatively small. Thus it is

important to use the adiabatic hypothesis at distances smaller than 4 Å. The velocity of the B atom in this case will be much smaller than the velocity of sound in W.

With the B atom already adsorbed in the smaller minimum at 4 Å it is possible to consider the cases when this atom can come closer to the surface. The deep minimum on the energy curve that is at the distance of ~ 1 Å to the W(110) surface means that if additional energy is applied to the B atom adsorbed in the energy minimum located at 4 Å, this atom may overcome the energy barrier between these minima. Thus the B atom will be removed from the surface in the outward direction or may be captured by the deeper energy minimum very close to the surface. This may occur also by the tunnelling of B, having a relatively small mass, through the corresponding potential barrier. The energy saving connected with this new location of the B atom is typical for chemisorption with extremely strong bonding of the B atom at the W(110) surface. So, the existence of an additional deep minimum means that it will be very difficult or almost impossible to 'clean' the W(110) surface with already adsorbed B atoms.

4. Summary

In our paper the results of the nonempirical study of the boron adhesion process on the (110) tungsten surface have been presented. A comparative analysis of the fine atomic structure in the vicinity of the surface clears up the behaviour of the system in the simulated adhesion process. The existence of a number of energy barriers in the adhesion path of the boron atom demonstrates the dependence of adhesion conditions on the energy of the atom approaching the surface. This result also shows that the conditions of the metalloid adhesion are influenced by the directional bonding nature and the structural reconstruction of the substrate surface.

The many-body interaction potentials were yielded in atomistic MC simulations of the boron adhesion process on the tungsten (110) surface. The accuracy of simulations was also checked. We have found out that the clusters containing 393 atoms are large enough to study adsorption modes for boron atoms.

We have demonstrated by direct calculations the influence of accounting for many-body interactions on the calculated energy characteristics of the adhesion path. We proved that the directional bonding between tungsten atoms in the vicinity of the (110) surface is a reason to form the favourable energy conditions for absorption of the boron atom at a distance of ~ 1 Å above the surface. Our results clearly show the changes of the energy of atoms in the system and the tendencies of the propagation of the elastic field in the vicinity of the (110) surface of W induced by the boron adhesion.

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