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### Short Communication

## A model of step geometry on the reconstructed W (001) surface

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**Abstract.** — The values of surface force constants indicate the presence of compressive surface stress on the ideal W (001) surface, supposing that surface interactions can be described by an effective two-body potential. Combining this idea with a phenomenological model of Roelofs *et al.*, we find that surface steps should expand at their edges and that the polarization of the reconstruction on the W (001) surface perpendicular to the step edge is preferred.

### 1. Introduction.

Properties of the stepped W (001) surface are not understood in detail. It was found that preferred orientation of the  $M_5 (\sqrt{2} \times \sqrt{2})R45^\circ$  reconstruction perpendicular to the step edge is induced at surface terraces. Nevertheless, the geometry at the step edges is not known [1, 2].

For semiconductor surfaces, a correlation between surface stress and step formation has been suggested [3]. On the other hand, a relation between the surface stress and surface force constants exists supposing that the surface force constants can be derived from an effective two-body potential acting between the surface atoms [4]. Let us repeat here the basic arguments. Consider two atoms placed at the distance  $r = a$  and interacting *via* the central two-body potential  $V(r)$ . For a small deformation the bond length change is  $\delta r \sim \delta_A + (2a)^{-1}\delta_B^2$ , where A, B denote the deformation parallel and perpendicular to the bond direction, respectively. Denoting  $\alpha = a^{-1}V'$ ,  $\beta = V''$  [5, 6] the derivatives of the potential, we find

$$\delta V \sim \alpha a \delta_A + 0.5\alpha \delta_B^2 + 0.5\beta \delta_A^2. \quad (1)$$

For symmetric surface geometries, the linear terms in equation (1) compensate mutually. Nevertheless, there is a surface stress proportional to  $\alpha$ . For structures with the symmetry broken, the linear term is generally restored. This idea was employed to describe the surface relaxation [7]. In the latter example, the bulk symmetry was broken by the surface formation.

For the ideal W (001) surface, the force constant  $\alpha_s$  describing interaction between the first surface neighbours is negative [5, 6] which points to the compressive (repulsive) surface stress

$\alpha_s a^2$  per surface unit cell [4]. As a consequence, nonzero net force at step edges causing their expansion can be anticipated [8].

Naturally, legitimacy of equation (1) and the use of surface force constant values at the step edge can be questioned. However, investigations [8-10] suggest that the very nature of interactions is common for many atomic arrangements (including steps) on W (001) and the repulsion originates from indirect (mediated by the metal) interactions. Hence, the equation (1) with the repulsive linear term should be correct qualitatively at least.

## 2. The model.

In the present paper, we use the phenomenological Hamiltonian of reference [11] fitted to reproduce the results of extensive first principles calculations [12]. One of its virtues is its simplicity since it is confined to the surface layer. To extract the  $\alpha_s$  value, however, an additional analysis is necessary. To this end, let us consider the harmonic part of the Hamiltonian [11]

$$0.5 \sum_i A u_i^2 + \sum_{(ij)} [J_1 \langle \mathbf{u}_i, \mathbf{u}_j \rangle + K_1 (u_{iA} u_{jA} - u_{iB} u_{jB})]. \quad (2)$$

Above,  $\mathbf{u}_i$  is the displacement vector at the site  $i$  parallel to the surface and A, B denote again the components parallel and perpendicular, respectively, to the bond  $(ij)$  between two nearest surface neighbours. The symbols  $(ij)$  and  $(ji)$  are treated as identical and should not appear twice in the sum. Finally, we do not include the very weak interaction ( $J_2$ -term [11]) between more distant neighbours in equation (2). Taking into account that every contribution  $u_i^2$  in (2) is shared by four bonds  $(ij)$ , we bring the harmonic part to the form

$$0.5 \sum_i (A + 4J_1) u_i^2 + 0.5 \sum_{(ij)} [(-J_1 - K_1) \delta_{ijA}^2 + (-J_1 + K_1) \delta_{ijB}^2 + 2K_1 (u_{iA}^2 - u_{iB}^2)]. \quad (3)$$

Here  $\delta_{ij} = \mathbf{u}_i - \mathbf{u}_j$ ,  $\delta_{ij}^2 = \delta_{ijA}^2 + \delta_{ijB}^2$ .

The first term is very small since  $A + 4J_1 \approx 0$  [11]. The last  $K_1$ -contribution is zero since for bonds  $(ij)$ ,  $(ik)$  mutually perpendicular,  $u_{iA}$  and  $u_{iB}$  interchange. From equation (1) we find  $\alpha_s = K_1 - J_1 = -63.28 \text{ mRy}/\text{\AA} = -0.86 \text{ eV}/\text{\AA}$ ,  $\beta_s = -K_1 - J_1 = -89.0 \text{ mRy}/\text{\AA} = -1.21 \text{ eV}/\text{\AA}$ . Absolute values of  $\alpha_s$ ,  $\beta_s$  we have obtained are somewhat higher than those of reference [6]. The latter property together with the fact that the interaction (3) is essentially decoupled from the rest of crystal are favourable for the reconstruction formation. The stability of the  $\bar{M}_5$  phase to rather elevated temperatures in the model [11] is perhaps explained by this remark. Of course, some coupling between the surface and bulk is described in [11] by the higher-order terms and by the  $z$ -dependent (surface relaxation) contribution. Let us note that description of the latter effect for W(001) is difficult [13].

Let us now explain the model of W(001) steps used below. The upper (001) terrace is modelled by a half-plane (or rather strip with a boundary condition) of atoms with the edge parallel to (10) and (11) direction, respectively. The Hamiltonian is exactly that of reference [11]. At edge atoms, however, the term  $F l_i$  is added, where  $l_i$  is the deformation perpendicular to the edge and  $F$  is the force derived from the linear term in equation (1). Besides that the  $A$ -term in (2) is common to four surface bonds and we use the value  $A(1-r/4)$  for edge atoms, where  $r = 1$  or  $2$  is the number of the bonds broken by the step formation. This change is rather unessential, however, since it reduces displacements at the step edge by  $0.01 - 0.02 \text{ \AA}$ . The half-plane is formed by atomic rows parallel to the edge. On the 14th (and following) row, the boundary condition assuming the  $\bar{M}_5$

reconstruction with the amplitude  $0.27 \text{ \AA}$  [11] is imposed. The period of the  $\bar{M}_5$  phase is two along the (10) rows and the same is supposed for the (10) step. For (11) chains, the  $\bar{M}_5$  period is one. However, to check the geometry proposed in reference [1] (Fig. 7), we allow the period two along the (11) direction, conserving at the same time the reflection plane symmetry perpendicular to the step edge. It appears, however, that the period obtained is one. To verify that the results arrived at are not influenced by the domain width, we checked that the edge geometry was not influenced by the boundary condition change (see below). Let us note that from the condition  $F_{iz} = 0$  for the force component at the site  $i$  perpendicular to the surface, vertical displacements can be excluded from the Hamiltonian reducing the number of degrees of freedom of the problem.

### 3. Results and discussion.

The results arrived at for the (10) and (11) step are presented in figure 1. We describe explicitly only those displacements, magnitudes and angles of which differ from the  $\bar{M}_5$  values more than about  $0.02 \text{ \AA}$  and  $2^\circ$ , respectively. In both cases, the upper terrace is expanded at the edge. The "ideal"  $\bar{M}_5$  structure is restored starting from the 4th atomic chain. The well resolved differences are found, however, at the edge for the (11) step and in two first rows in the (10) case.

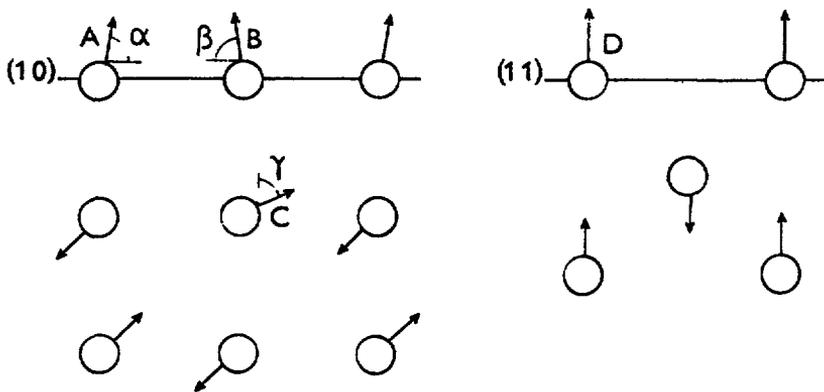


Fig. 1. — Surface atom displacements at the (10) and (11) step edges on the W(001) surface. Values of selected displacement magnitudes and angles are given:  $0.33 \text{ \AA}$  (A),  $0.32 \text{ \AA}$  (B),  $0.23 \text{ \AA}$  (C),  $0.41 \text{ \AA}$  (D),  $82^\circ$  ( $\alpha$ ),  $81^\circ$  ( $\beta$ ),  $64^\circ$  ( $\gamma$ ).

For the (11) terrace, it is possible to impose two different boundary conditions with improper  $\bar{M}_5$  polarization on the 14th row. First, we take the polarization parallel to the step edge. In the second case, the transversal polarization is oriented towards the edge which prevents regular alternation of the deformation sign when going from the expanded step edge. In the former case, a domain wall with energy  $6 \text{ mRy}$  per one step along the atomic row and of width 4-5 rows is formed; in the latter case, the width and energy are half the values just quoted. Of course, similar structures can be stable only supposing they are pinned by defects or adsorbates. The geometry at the edge is not influenced by the boundary condition choice. The examples considered indicate that 1) the orientation of deformation transversal to the step edge is clearly preferred and, 2) the diameter of the region influenced by various kinds of defects can vary from case to case.

To summarize, it is suggested that the reconstructed domains on the W(001) surface expand at step edges as a result of compressive surface stress. The specific geometric features are confined to 1-2 atomic rows and transversal orientation of the reconstruction is preferred for the (11) step.

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