

A computational study of hcp Ti and Zr stepped surfaces

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Abstract The structure and energetics of ledge pairs (atomic steps) in surfaces (0001), (10 $\bar{1}$ 0), (1210) of hcp Zr and Ti are studied by computer simulation using embedded-atom-type interatomic potentials. The configurations considered are the face-to-face, back-to-back, sequential, and double, according to their cross-sectional view. Ledge and kink formation and interaction energies are obtained. Vacancies and adatoms are introduced to study their formation and migration energies in interaction with the ledges. But for one case (surface (10 $\bar{1}$ 0)) it is found that ledges are preferred sites for vacancy and adatom formation; also, their overall effect on diffusion is predicted to be small. The results indicate that the effect of ledges can be neglected beyond a few atomic distances.

Introduction

Surface diffusion is a fundamental process in many surface phenomena, such as crystal growth, sintering, corrosion and surface chemical reactions. Numerous experimental and theoretical efforts have been attempted to understand the fundamentals of surface

diffusion. In most of these studies the theoretical tools employed are still based on the terrace-kink-ledge (TKL) model laid down by Burton et al. in the 50's [1–4].

The great majority of the theoretical studies in the literature dealing with ledges, kinks, and their interactions with point defects, refer to the cubic structure. In one of the pioneering works, Wynblatt [5] used Morse pair potentials to simulate isolated steps on Cu (001); he considered several configurations for ledge pairs and calculated their interaction as a function of separation predicting short-range repulsive forces. This interaction was shown to follow an inverse square dependence in a more recent work by Shilkrot and Srolovitz [6], who simulated Ni and Au surfaces by means of embedded atom method (EAM) interatomic potentials. They also elaborated an elastic model on those grounds; the interaction however was of very small magnitude.

Closer to diffusion, Liu and Adams [7, 8] used EAM potentials to study stepped surfaces in Ni, Cu, and Ag for several surface and ledge orientations, claiming agreement with STM and X-ray diffraction measurements. They computed formation energy of ledges and kinks finding that the former is lower and the latter higher as the atomic row forming the ledge becomes more compact. They also obtained migration energies for adatoms jumping along the ledges, predicting a strong dependence upon orientation and that their presence may enhance surface diffusion. With similar techniques, Nelson et al. [9] calculated formation energies of single and double steps, and kinks for surfaces (100) and (111) in Ag as well as diffusion barriers for vacancies and adatoms in their neighborhood. They found a small effect on vacancies whereas barriers for

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adatoms were sizably diminished with respect to the terrace.

Regarding the migration mechanisms themselves, Villarba and Jónsson [10] used EAM to model adatom migration on Pt surfaces finding two possible mechanisms, hop and exchange; also, steps were predicted to be adatom traps at low enough temperatures. Similarly, Ferrando and Tréglia [11] used N-body tight-binding potentials and quenched molecular dynamics to investigate adatom migration near steps on the (111) surface of Ag and Au. They found that adatom descending jumps can be of the exchange as well as hop type, while their energy barriers depend on the step considered. Máca et al. [12] also used N-body tight-binding potentials in a detailed study of adatom migration on the Pt (111) surface. Adatoms descending from straight steps, steps with kinks, and small islands as well as jumping along these structures were considered. They predicted the minimum energy process to be an exchange for a descent near a kink or an island's corner. Besides, for the two microfacets possible for ledges along $\{110\}$, namely $\{111\}$ and $\{100\}$, migration along the $\{111\}$ one was found to be faster.

Surfaces of the hcp structure have been far less studied in the past [13, 14] despite of the technological relevance of materials such as α -Zr and α -Ti. From a more fundamental point of view, some similarities with the cubic structure may be expected but also some differences, stemming from the crystal basis of two non-equivalent atoms. Among the extant experimental literature on steps, Dulub et al. [15] employed LEED, LEIS, and STM to study the geometric and electronic structure of (0001), (000 $\bar{1}$), (10 $\bar{1}$ 0), and (11 $\bar{2}$ 0) surfaces in ZnO single crystals. They demonstrated that terraces are limited by fluctuating steps at finite temperatures; their other findings are however difficult to assess in the face of hcp metals, because ZnO is a semiconducting substance of the wurzite structure, showing polarity effects, mixed bonds effects, etc.

In the present work we apply molecular statics and EAM-type interatomic potentials to study step and kink formation energies, step–step interactions, and migration of adatoms and vacancies parallel and perpendicular to the step edges, in α -Zr and α -Ti surfaces. The task was already initiated in previous works [16–18] limited however to the terraces only, i.e., (0001), (10 $\bar{1}$ 0), (1 $\bar{2}$ 10). The paper is then organized as follows: Section 2 describes the calculation procedures, Section 3 presents the results separately for the three surfaces considered, finally Section 4 advances our conclusions.

Calculation method

Steps are build starting from two crystallites in the form of parallelepipeds of respective heights z and $z + \Delta z$ and minimum periodic dimensions on the surface plane (x, y). Both have been previously energy-relaxed under cyclic boundary conditions parallel to the surface and rigid conditions at the bottom plane. By repetition and matching of these elemental blocks, the simulation crystallite for a step of height Δz is obtained as illustrated in Fig. 1; the sizes are about 20 planes deep into bulk, 21 planes wide, and 30 periodic lengths along the step direction. Only steps along the most compact direction on each surface are studied, i.e., $\langle 1\bar{2}10 \rangle$ on (0001) and (10 $\bar{1}$ 0), and $\langle 0001 \rangle$ on (1 $\bar{2}$ 10).

Figure 2 shows a cross-section view of the ledge pairs considered, so called (after [5]) as sequential (S), face-to-face (F), and back-to-back (B). Their formation energy is computed according to,

$$E^f = E - (E_S \mp NE_{\text{coh}}), \quad (1)$$

where E/E_S is the (relaxed) energy of the crystallite with/without steps, and the last term compensates for the difference in the number of atoms N , being E_{coh} the cohesive energy. We note in passing that on the basal surface the constituents of the ledge pairs are of different kind (coordination), because for crystallographic reasons it is impossible to form pairs of the same kind.

The EAM-type interatomic potentials for Ti and Zr developed in [19, 20] and used in former works [16–18] are employed here for the energy computations. Briefly, they reproduce the experimental values of both lattice parameters a and c , the five elastic constants, the cohesive energy, and an approximate unrelaxed vacancy formation energy.

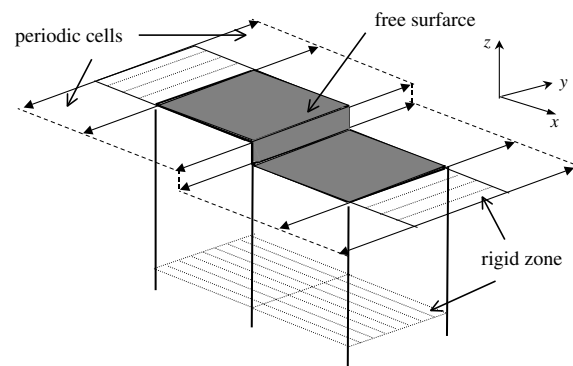
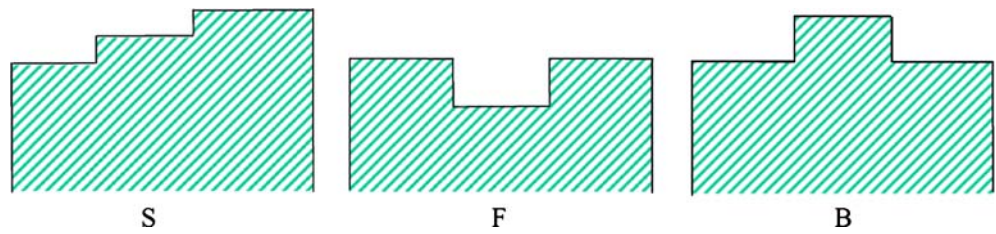


Fig. 1 Scheme of the simulation crystallite showing the step building process

Fig. 2 Cross-section view of interacting step-pairs and naming conventions



Once the step is build, point defects are introduced in nearby positions following standard procedures, namely, an atom is taken away from a lattice node (vacancy) or deposited onto the surface (adatom). Their formation energy is obtained following a similar recipe as in Eq. 1 where E/E_S refer now to the energy of the stepped surface with/without the point defect ($N = 1$). Regarding migration, the procedures detailed in [16] are applied for the barrier calculations. Vacancies move on terraces through single or multiple jumps, they can also bridge terraces by hopping or multiple jumps [7, 10, 21–23], the latter involving several atoms (normally two) at the same time. Adatoms move on terraces by single or exchange jumps and can bridge terraces by hopping or exchange, the latter involving the coordinated motion of two atoms. Irrespective of defect type and jump mechanism, the saddle point configurations (activated states) are obtained by minimizing the system energy within the hyperplane

of dimension $(3n - 1)$ — n is the number of moving atoms—perpendicular to the reaction coordinate. This coordinate is defined by the controlled displacement of a unique atom that drives the jump [18].

Results

Surface (0001)

As advanced before, two kinds of single steps are distinguished so called T1 and T2, whose top view is depicted in Fig. 3. Clearly, the coordination of atoms in T2, Fig. 3b, is higher than in T1, Fig. 3a. Accordingly, sequential steps are named as S_{T1-T2} and S_{T2-T1} if the upper step is of T1 or T2 kind respectively; when close enough these form the double steps D_{T1-T2} and D_{T2-T1} .

Table 1 reports the formation energies of the ledge pairs. This is very close to a constant number, gathered

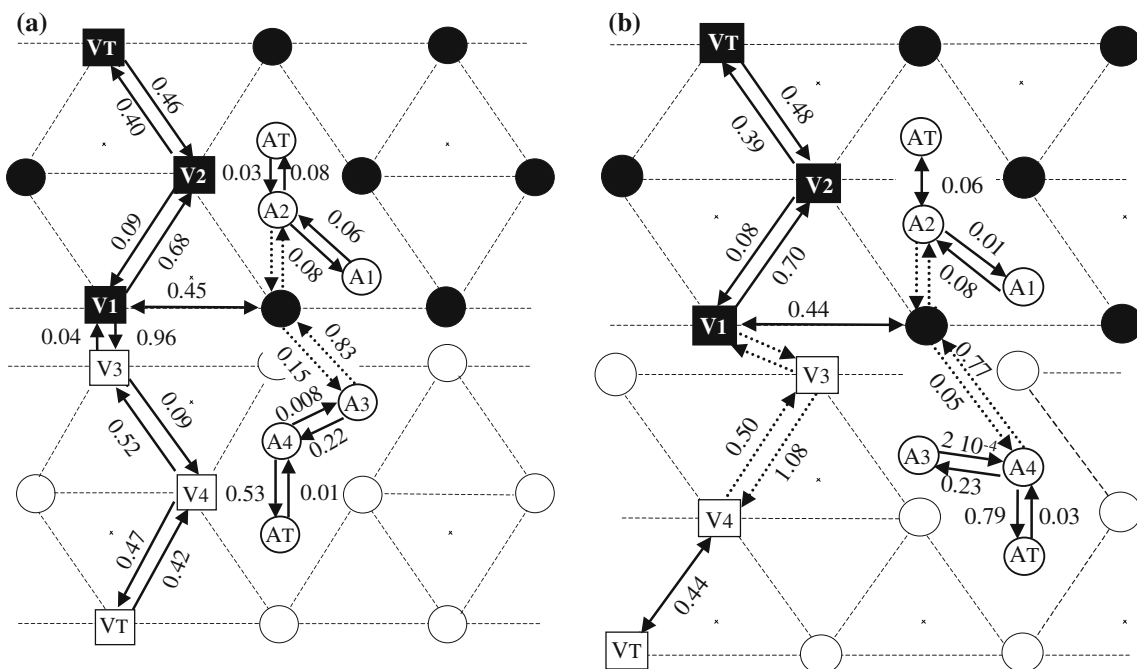


Fig. 3 Top view of step edges on the (0001) surface: (a) T1-type step, (b) T2-type. Full/empty circles stand for upper/lower terrace sites; vacancy/adatom sites indicated with V_i/A_i ;

full arrows depict single jumps, dotted arrows multiple or exchange ones. The numbers indicate migration energies calculated for T1

Table 1 Calculated ledge pair formation energies (eV/*a*) for surface (0001)

	P	D_{T2-T1}	D_{T1-T2}	F_1	B_1
Ti	0.58	0.60	0.54	0.57	0.66
Zr	0.61	0.66	0.57	0.61	0.66

under column P, irrespective of their separation unless it is minimum, in which case the double steps or the limiting cases F_1 and B_1 (for one atomic row) are formed. The results indicate a very short-range interaction, slightly repulsive for D_{T2-T1} and B_1 and attractive for D_{T1-T2} and F_1 .

Regarding the interaction with the point defects, Fig. 3 shows the positions for the vacancy (V_i) and the adatom (A_i) that have been considered in Ti. Adatom equilibrium positions in Zr terraces are slightly different than in Ti [16], however close to steps both adopt similar configurations. Although not clearly shown in the figure, the step slightly modifies the adatom equilibrium sites on the terrace; these are however recovered at about two atomic distances from the step [18]. Also, for both steps note positions V_1 , A_3 and A_4 that give rise to kinks.

Table 2 reports the formation energies of the vacancies and adatoms depicted in Fig. 3; all other sites in practice require the same energy as for terraces (VT and AT respectively). The results show a clear tendency to kink formation, being adatom kinks (A_3 and A_4) slightly more energetic (6% in average) than vacancy ones (V_1). As for steps, kink-kink interaction is very short ranged: The formation energy of B-type kink pairs remains constant irrespective of their separation, increasing about 10% when the later is minimum (A_3 and A_4 sites for T1 and T2 respectively), whereas for the F-type ones no significant changes were detected. Worth of noticing is the relatively high energy value required to form vacancies in V_3 sites, which can be traced to the higher coordination of the atom involved.

Figure 3 also shows the main jumps studied for both point defects; solid lines indicate single jumps connecting start and end positions, dotted lines correspond to multiple/exchange jumps passing through intermediate sites. Both materials show essentially similar behaviors, so we concentrate on Ti and give the corresponding values for Zr within parenthesis when

pertinent. Because we want to address the step effects on migration relative to the terrace, it is important to keep in mind the corresponding migration energies to be used as reference values; these are 0.06 eV (0.02 eV) for adatoms and 0.45 eV (0.44 eV) for vacancies.

Adatoms in the T1 step descend from upper terraces via an exchange jump, its energy being 0.15 eV (0.09 eV). This value is higher than the reference giving rise to a repulsive (so called Shwoebel [24]) barrier. In the lower terrace they are attracted by the step, jump $AT \rightarrow A_4$ having a lower barrier, 0.01 eV (0.02 eV) than the converse one, 0.53 eV (0.77 eV). Once in A_4 the jump towards A_3 is essentially athermal, 0.008 eV (0.01 eV) being this a trapping site. Then the step is lightly reflective on the upper terrace and absorbing on the lower one, effect that decays beyond a few atomic rows. On the other hand, jumps parallel to the step entail higher barriers than on the terrace, 0.22 eV (0.16 eV), so that the overall effect of this step on adatom motion is surely not one of enhancing migration.

Focusing now on the vacancy for the same step, though there is a very small barrier to reach V_2 sites on the upper terrace, once there the jump to V_1 is fairly easy, 0.09 eV (0.09 eV). A minimal kink pair is then formed wherefrom basically 1-dimensional motion is the only possibility; the corresponding energy, 0.45 eV (0.38 eV), being about the same as the reference value. On the lower terrace, vacancies are very slightly attracted to sites V_4 ; once there however the jump $V_4 \rightarrow V_3$ requires higher energy than on the terrace, 0.52 eV (0.77 eV). Position V_3 , of high formation energy, is unstable; from there the vacancy migrates to V_1 via a hop with 0.04 eV (0.02 eV) or backwards to V_4 with 0.09 eV (Ti only).

Regarding adatoms in step T2, from A_2 sites in the upper terrace two jumps are possible, a single $A_2 \rightarrow A_1$ requiring 0.01 eV (0.02 eV) or a descent by exchange towards A_4 with 0.05 eV (0.009 eV);

Table 2 Vacancy and adatom formation energies (eV) for the positions in Fig. 3, surface (0001)

	Step	A1	A2	A3	A4	A5	AT	V1	V2	V3	V4	VT
Ti	T1	1.09	1.03	0.35	0.56	—	1.08	0.32	0.91	1.24	0.81	0.85
	T2	1.09	1.03	0.54	0.31	—	—	0.29	0.91	1.37	0.87	—
Zr	T1	1.12	1.07	0.36	0.52	1.11	1.11	0.33	0.93	1.32	0.83	0.87
	T2	1.10	1.25	0.54	0.35	1.07	—	0.32	0.94	1.44	0.94	—

contrary to the T1 case no repulsive barrier is found. As before, the lower terrace side is attractive for adatoms, jump $AT \rightarrow A4$ requiring a fairly smaller energy than the converse, 0.03 eV against 0.79 eV (0.02 eV, 0.72 eV). The most probable escape jump from this trapping site is to A3 with 0.23 eV (fairly larger than the reference), though the converse jump is essentially athermal. A small difference appears between Ti and Zr in that, for the latter, migration energies on the lower side and parallel to the step are lightly smaller than on the terrace. In summary, no significant migration enhancement is predicted either in this case.

The description for the vacancy in the T2 step is very similar to the one already given for the T1 case. A difference appears in that vacancies in the lower terrace V4 sites reach V1 sites in kink positions through a multiple jump involving V3; this difference however is not to be stressed owing to the instability of V3 sites on T1 steps.

Surface $(10\bar{1}0)$

Two endings are possible for this surface, so called $(10\bar{1}0)_s$ and $(10\bar{1}0)_c$ according to the distance between first and second plane being $a/\sqrt{3}$ or $a/2\sqrt{3}$ respectively. Ending “c” is however fairly lower in energy than “s” [17], so that the minimum energy step configuration was found to be one of double height with both bounding terraces of the “c” type; it is depicted in Fig. 4 while the corresponding formation energy is reported in Table 3 column D. The figure also shows a couple of “excited” configurations obtained by extracting one (D’) or two (D’’) atoms from the upper terrace step edge, the corresponding energies being reported in Table 3. One may think of this excited

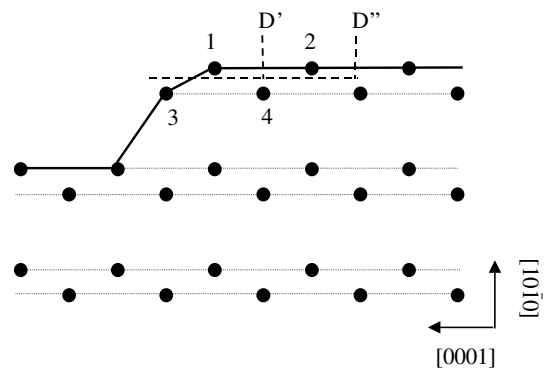


Fig. 4 Cross-section view of minimum energy step structure on $(10\bar{1}0)$ surface. See main text for details

configurations as a (virtual) way of exposing surface ending “s” at the expense of “c”. In fact this expectation is fulfilled even at the very early stage of D’ and D’’, given that their energy difference of 0.25 eV/a is in coincidence with the energy difference between the two surface endings. Such an outcome can then be turned into a method of unraveling “true” step–step interaction effects by subtracting surface contributions [25]. Table 3 also reports the formation energies for pairs of D steps in configurations F, B, and S; as before, the interaction is very short-ranged if existent at all.

Figure 5 depicts the vacancy and adatom sites, V_i and A_i respectively, that were considered in the neighborhood of step D, while their formation energies are reported in Table 4. For both materials position V1 in the upper terrace edge is lightly more energetic than those well inside the terrace (VT), the other positions frankly within the step, V3 and V4, are of considerably higher energy indicating a repulsive character. Regarding adatoms, sites within the step, A1 and A5, are of fairly larger energy than terrace sites (AT)

Table 3 Calculated step formation energies (eV/a) for surface $(10\bar{1}0)$

	D	F	B	S	D'	D''
Ti	0.086	0.172	0.172	0.172	0.247	0.497
Zr	0.090	0.180	0.180	0.180	0.320	0.556

Fig. 5 Top view of step edge on the $(10\bar{1}0)$ surface. Description is similar to Fig. 3 but for shaded symbols indicating middle plane step sites, and dotted squares (V6, V7) meaning sub-surface plane vacancy sites

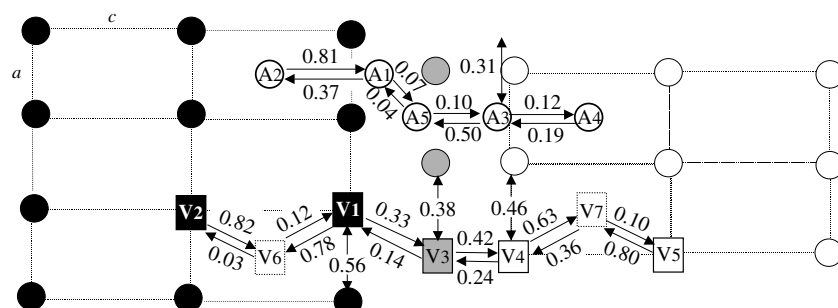


Table 4 Vacancy and adatom formation energies (eV) for the positions in Fig. 5, surface $(10\bar{1}0)$

	A1	A2	A3	A4	A5	AT	V1	V2	V3	V4	V5	V6	V7	VT
Ti	1.14	0.70	0.78	0.70	1.16	0.70	0.51	0.45	0.70	0.88	0.45	1.18	1.16	0.44
Zr	1.24	0.68	0.85	0.70	1.24	0.68	0.51	0.46	0.73	0.93	0.47	1.23	1.22	0.46
														1.24

Second rows indicate vacancies in the second plane

whereas for all the other sites shown the energy is about the same or slightly higher. Again, as found above, the step effects are basically lost at a distance of about two atomic rows.

Figure 5 also reports the jumps and migration energies for Ti, similar values were found for Zr. Generally, jumps towards the step are unfavored with respect to the ones in the reverse sense; vacancy migration however is predicted to be somewhat faster once within the three atomic rows forming the step (0.60 eV is the terrace value [18]). Adatoms on the other hand, can jump within the step following a zigzag shape path $A1 \rightarrow A5 \rightarrow A1$ at slightly lower energies than required on the terrace (0.08 eV); also, jumps perpendicular to the step are faster than the corresponding ones on the terrace (about 0.8 eV) particularly on the lower side, much slower though than the parallel jumps. In summary, the presence of this type of step seems to somewhat enhance point defect migration.

Surface $(1\bar{2}10)$

From the crystallographic point of view two single-height steps may be considered on this surface, here called Tm and Tb; Fig. 6 depicts the corresponding cross-section views. The figure clearly shows Tm is a better coordinated structure so that a lower formation energy may be expected, in agreement with the values reported in Table 5 (columns Tm, Tb). On the other hand, possible interacting pair profiles are depicted in Fig. 7 with corresponding formation energies reported in Table 5. As in previous findings, the step-step interaction is very short-ranged; moreover, any structure involving the “b”-type edge is of relatively higher

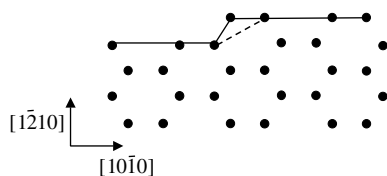


Fig. 6 Cross-section view of possible single-height steps on the (1210) surface: Tm/Tb solid/dashed line

energy than those made out of only “m”-type edge, so our analysis below will be restricted to this kind of structure.

Figure 8 shows a Tm top view with the vacancy and adatom sites that were considered, their formation energy being reported in Table 6. Sites A4 and V1 possess lower formation energy than terrace values (AT, VT respectively) in both metals, indicating a tendency to form kinks. Of note is the large formation energy in site V3 that particularly for Ti corresponds to an unstable configuration.

Adatoms are slightly attracted to the step on the lower terrace (towards site A4) and can bridge the step by means of an exchange jump, $A1 \leftrightarrow A3$, though only by surmounting a fairly large energy barrier (smaller for the descent). Even though the latter is somewhat larger than the corresponding exchange jump on the terrace (0.56 eV in Ti, [18]), the effect on the overall adatom migration is however expected to be small, owing to the high anisotropy favoring parallel motion.

Regarding the vacancy, it was demonstrated that effective 2-dimensional motion on this surface requires the intervention of sub-surface planes [18] (beyond the fourth for well converged diffusivities) where the vacancy encounters unstable configurations, (therefore Table 6 does not report formation energies for them). The step is no exception to this behavior and in fact the relative abundance of multiple jumps is a consequence of it. Of note however for the step situation is that, overall, the migration energies involved are somewhat smaller than within the terrace (0.35 up to 1.72 eV for jumps including the first two planes only), so a small enhancement of the diffusivity may be expected.

Summary and conclusions

We have employed computer simulation techniques furnished with semi-empirical many-body interatomic potentials in order to assess mainly how steps on surfaces of the hcp metals Zr and Ti may affect atomic migration.

Table 5 Calculated step formation energies (eV/c) for surface (1210)

	Tm	Tb	F _{mm} B _{mm} S _{mm}	F _{bm} B _{bm} S _{bm}	F _{bb} B _{bb} S _{bb}	D _{bm}	D _{mb}	D _{mm}	D _{bb}
Ti	0.04	0.31	0.08	0.35	0.63	0.57	0.72	0.08	0.59
Zr	0.06	0.33	0.13	0.40	0.67	0.62	0.77	0.13	0.63

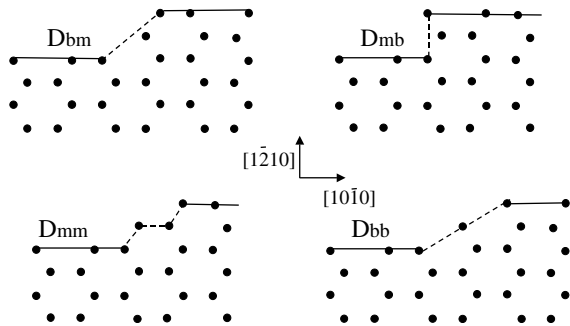


Fig. 7 Cross-section view of possible double-height steps on the (1210) surface

Similarly to the (111) surface of the fcc structure, two single height step types of different coordination were found on the basal surface. They can merge in an energetically slightly favored double height step D_{T1-T2} that despite of having the same coordination as the D_{T2-T1} , but different topography, is of lower energy. This is in contrast with the results for the fcc (111) surface, where the energy difference among the two structures stems from different coordination [9]. On the surface (1010) single height steps are energetically

unfavored, due to large differences in the energy of the two possible surface endings; a double step structure is formed instead in the boundary of two low energy terraces. On the (1210) surface two single height steps are possible, however their difference in coordination causes a relatively large difference in energy, then favoring one of them. In all the cases studied the interaction among steps was found to be negligible.

In agreement with previous studies on the fcc structure [10, 12] and with the assumptions of the theory of crystal growth (e.g. in [26]), we find that kinks can easily form on steps by interaction with point defects; this interaction however is of very short range, one or two atomic rows from the step edge. Previous studies on fcc metals using many-body interatomic potentials [27] predicted the adatom migration to be much faster along the step than on the terrace. In contrast, our results for the basal surface show no appreciable influence if on the upper terrace, or some small negative/positive effect (Ti/Zr T2 step) if on the lower terrace. Some migration enhancement was also found for both, adatoms and vacancies, in the D step of the (1010) surface, and no influence or a slight detriment for the Tm step of the (1210) surface.

Fig. 8 Top view of step edge on the (1210) surface. Description is similar to previous cases. Empty squares stand for sub-surface vacancies

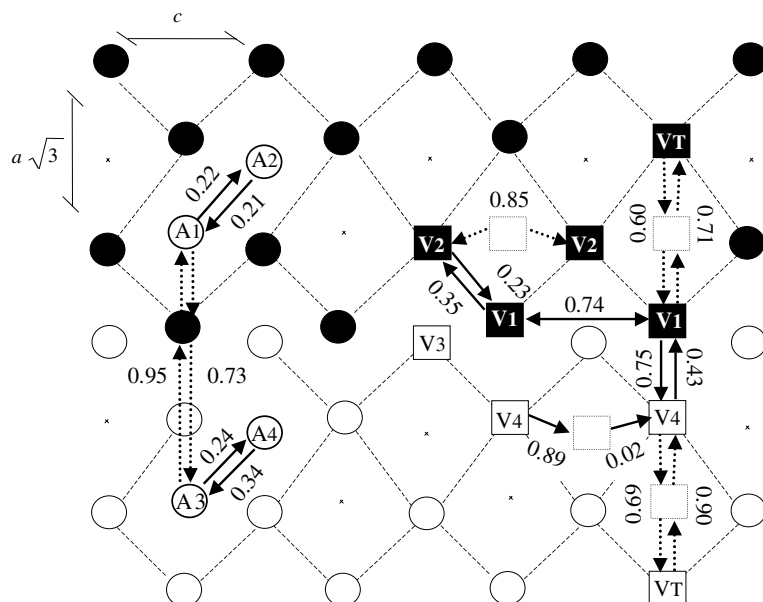


Table 6 Vacancy and adatom formation energies (eV) for Tm step of surface (1210)

	A1	A2	A3	A4	AT	V1	V2	V3	V4	VT
Ti	0.33	0.34	0.35	0.26	0.39	0.24	0.36	—	0.56	0.34
Zr	0.39	0.39	0.41	0.27	0.33	0.25	0.43	1.29	0.63	0.41

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