PLANAR DEFECTS ON {121} PLANE IN 2H STRUCTURE

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The type I twinning is observed in {121} plane in the martensite with 2H structure. This type of martensite arises often in the Cu-based shape memory alloys. The structures of stacking faults and twin boundaries on {121} plane in 2H structure are modelled by using of many-body potentials of Finnis-Sinclair type. Two types of stacking faults and three types of twin boundaries were found as result of calculation.

INTRODUCTION

Shape memory alloys are intensively studied during last years. These materials exhibit a variety of deformation processes derived from martensitic phase transformation. Twinning in shape memory alloys is interesting and important field for investigation. The twinning in the 2H martensite is considered in this paper. The 2H martensite is observed in Cu-based alloys such as Cu-Al-Ni, Cu-Al-Zn, Cu-Al-Mn. The B19 phase in Ni-Ti possesses the 2H structure as well. The 2H structure possesses orthorhombic lattice, which can be recognized as close packed hexagonal if ordering is disregarded in binary or ternary systems.

Three types of twins are observed in systems with the 2H structure. For instance, there are compound twins on a $\{101\}\gamma_1'$ plane, type-I twins on a $\{121\}\gamma_1'$ plane and type-II twins on an irrational plane near $\{231\}\gamma_1$ [1-3] in Cu-Al-Ni. It was found that the large difference exists between the critical resolved shear stresses for type-II (7MPa) and compound twinning (0.7MPa) in 2H martensite of Cu-Al-Ni alloy [4]. The similar trend (i.e higher resolved shear stress for type-II twinning than for compound twinning) was found in Cu-Al-Mn alloy but difference is smaller in this material [5]. Critical resolved shear stress for type II twinning is 15 MPa and for compound twinning 10 MPa in the last case.

The {121} plane in 2H structure is a plane of type I twinning and it corresponds to the pyramidal $\{10\bar{1}1\}$ twinning in the hcp lattice if ordering in binary or ternary systems is disregarded. The $\{10\bar{1}1\}$ twin boundaries are formed for instance in the process of bcc-hcp transitions in Ti and Ti-Al alloys [6]. The {121} twinning is observed in the 2H martensite of copper-based alloys such as Cu-Al-Ni [7] and Cu-Al-Zn [8]. It was found by HREM observation that a stable configuration of the {121} orthorhombic boundary is defined by a single plane of atoms, formed by coalescence of two adjacent to boundary planes of atoms [8].

In order to understand difference in the behaviour of twinning modes it is necessary to know structures of twin boundaries. The knowledge about stacking faults structure in the twinning plane can be useful for understanding of twin nucleation and growth processes. The modelling of simple interfaces in the {121} plane in 2H structure is performed in present work. The structures of twin boundaries and stacking faults are considered. Finnis-Sinclair type many-body potential, which was proposed originally by Rosato [9] for fcc transition metals, was selected for calculations in this work. This potential was chosen mainly for its relative simplicity - it contains only five parameters. The aim of this paper is not to describe

interfaces in specific materials but to calculate their structure by using of several potentials in order to find trends how interface structure depends on interatomic potentials.

MODEL

The many-body potential (1) was taken in a simple analytical form with only five parameters A, ξ, p, q, r_0 proposed in [9]

$$U = -\sum_i \left(E_b^i + E_r^i \right)$$

$$E_b^i = -\left\{ \sum_j \xi^2 \exp\left[-2q\left(\frac{r_{ij}}{r_0} - 1 \right) \right] \right\}^{\frac{1}{2}} \tag{1}$$

$$E_r^i = \sum_j A \exp\left[-p\left(\frac{r_{ij}}{r_0} - 1 \right) \right]$$

In order to obtain reasonable scaling of energy and distances the coefficients A and ξ were fitted to the cohesive energy and lattice parameter of silver. The parameters p and q were changed freely to alter the properties. The parameter r_0 was taken equal to the first neighbors separation: $r_0 = a_0 / \sqrt{2}$. Each part E_r^i and E_b^i were cut on the distance corresponding to the 3rd neighbours of fcc lattice. Between the distances of the 3rd neighbours (r_3) and 4th neighbours (r_c) the expressions for E_r^i and E_b^i were replaced by a fifth order polynomials

$$E_b^i(r) = \alpha(r - r_c)^5 + \beta(r - r_c)^4 + \gamma(r - r_c)^3, r > r_3 \tag{2}$$

$$E_i^b(r) = \alpha_1(r - r_c)^5 + \beta_1(r - r_c)^4 + \gamma_1(r - r_c)^3, r > r_3 \tag{3}$$

Three potentials, which manifest qualitatively different behaviour, were chosen for further investigation. The parameters of these potentials are $p=9$ and $q=1$, 1.5 and 2. We will designate these potentials as p9q1, p9q1.5 and p9q2 respectively. The stability of such potentials was analysed also in [10]. The most stable structures are bcc and hcp with non-ideal c/a for p9q1 and p9q1.5 potentials, respectively, and fcc is the most stable structure for p9q2 potentials. The parameters of used potentials are listed in Table 1.

The blocks of ~ 30000 atoms were used for calculation of energies and structures of interfaces. Three type of calculations were performed by means of LAMMPS program [11, 12], i.e. the calculation of unrelaxed structure energy, calculation with atomic position relaxations in the direction perpendicular to the interface and energy relaxations with movement of atoms allowed in all directions.

STACKING FAULTS

The generalized stacking faults represent theoretical constructs where one part of the crystal is displaced with respect to the other part on certain crystallographic plane. The energy dependence of such fault on the displacement vector is called γ-surface. The concept of γ-surface was introduced in works by Vitek [13, 14].

Since two types of {121} interplanar distances occur two types of γ-surfaces are considered. We call the first one as narrow-type i.e. the crystal is cut between the close planes, and the second type we call as wide-type, i.e. the crystal is cut between the planes with

larger interplanar distance. It is necessary to note that two {121} planes with smaller interplanar distance are considered in the literature as one corrugated plane [8]. Let us mark two alternate {121} planes with the small interplanar distance as α and β, respectively. The planes α and β form a corrugated {121} plane together (see Fig. 5). A pair of planes with the smaller interplanar distance is meant as one {121} plane in the text below.

Table 1 Parameters of many-body potentials. r_0=2.892066736 for all potentials. The intervals where potentials is replaced by polynomial between third neighbours distance r_3=5.0092065 and cut-off radius r_c=5.7841334 are same for all potentials too. A, ξ are potentials parameters and α, β, γ, $α_1$, $β_1$, $γ_1$ are parameters of polynomials (2) and (3). The parameters units are selected in a way to obtain energy in eV and distances in Å.

	p9q1	p9q1.5	p9q2
A	0.038952362	0.05774643615	0.0774808638
ξ	0.762446703	0.90205767	1.0250236
α	-2.1823642	-1.2668815	-0.67556849
β	-4.3010659	-2.51468371	-1.3475536
γ	-2.3114016	-1.3824144	-0.75934542
$α_1$	$-3.2094594 \cdot 10^{-4}$	$-4.7579872 \cdot 10^{-4}$	$-6.3839949 \cdot 10^{-4}$
$β_1$	$-5.8489251 \cdot 10^{-4}$	$-8.6709653 \cdot 10^{-4}$	$-1.1634205 \cdot 10^{-3}$
$γ_1$	$-3.7570877 \cdot 10^{-4}$	$-5.5698400 \cdot 10^{-4}$	$-7.4732927 \cdot 10^{-4}$

Table 2 Locations and energies of (121) stacking faults

	A	E(A), eV/Å^2	B	E(B), eV/Å^2
p9q1	$0.069[23\bar{8}]$	0.025	$0.189[23\bar{8}]$	0.015
p9q1.5	$0.068[23\bar{8}]$	0.023	$0.191[23\bar{8}]$	0.017
p9q2	$0.060[23\bar{8}]$	0.020	$0.193[23\bar{8}]$	0.016

The block with periodical conditions in the $[\bar{2}10]$ and $[23\bar{8}]$ directions was considered. These directions lie in the (121) orthorhombic plane and they are perpendicular two each other. No minimum corresponding to a stacking fault is found in the "narrow type" γ-surfaces. But two types of "wide-type" stacking faults were found. The topology of γ-surfaces is similar for all potentials. The γ-surface for p9q1.5 potential is shown in Fig. 1 as an example. Two types of stacking faults are marked as A and B. The cross-sections of γ-surfaces at 0 and $1/8[\bar{2}10]$ are the same but the last one is shifted by $1/8[23\bar{8}]$. The locations of stacking faults are different for different potentials. These locations are listed in Table 2 as well as stacking fault energies. $[23\bar{8}]$ cross-sections of (121) γ-surfaces are shown in Fig. 2 for p9q1, p9q1.5 and p9q2 potentials. Letters A and B mark stable stacking faults.

Fig. 3 and 4 represent type A and B stacking faults for p9q2 potential respectively. Relaxations were performed in the direction perpendicular to the (121) plane. The corrugations becomes smaller for the closest to the fault (121) planes for both types of faults. The fault A can be approximately interpreted as a fault with extra (121) plane i.e. the extrinsic fault (Fig.3). In a similar way the fault B can be considered as a fault with the missing (121) plane i.e. the intrinsic fault (Fig. 4).
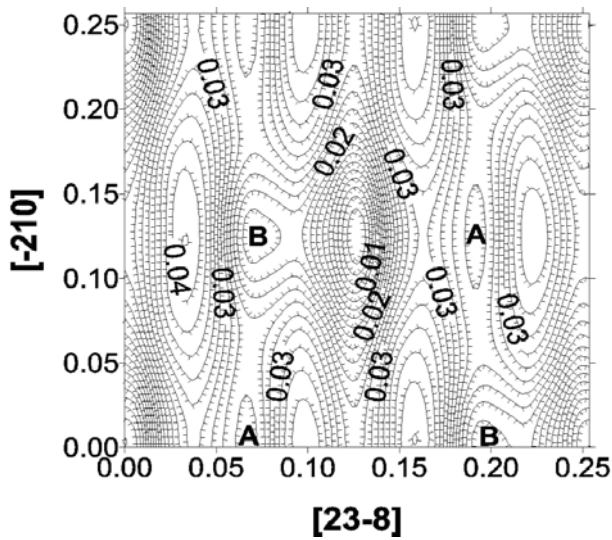
Fig. 1 *(121) 2H γ-surface for p9q1.5 potential. Stable stacking faults are marked by letters A and B. Hachures are shown in the downhill direction.*
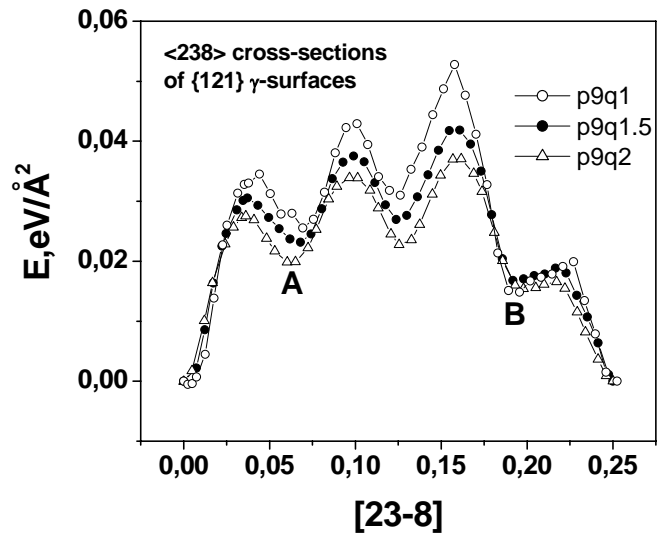
Fig. 2 $[23\bar{8}]$ *cross-sections of (121) γ-surfaces for p9q1, p9q1.5 and p9q2 potentials. Stable stacking faults are marked by letters A and B. The third minimum between A and B correspond to inflexion point.*
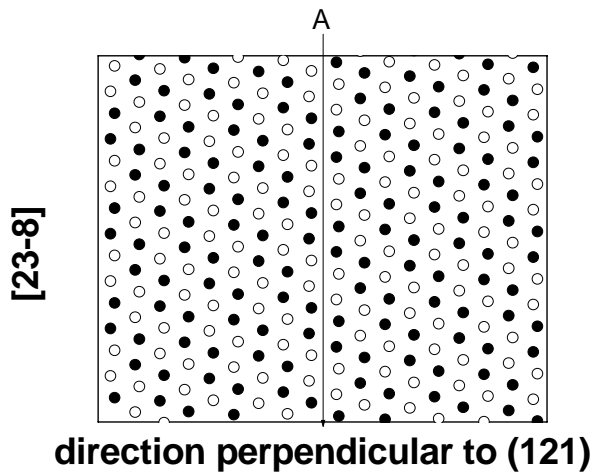

Fig. 3 *Type A (121) stacking fault for p9q2 potential. Projection in the $[\bar{2}10]$ direction. Black and white circles represent atoms in two alternate planes parallel to the projection plane.*
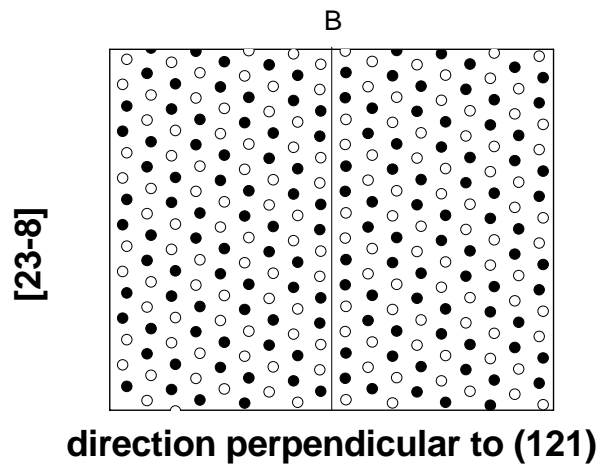
Fig. 4 *Type B (121) stacking fault for p9q2 potential. The same notation as in Fig. 3.*

nes αβ we can construct three types of twin boundaries with mirror symmetry. Let us denote them as Twin I, Twin II and Twin III as follows:

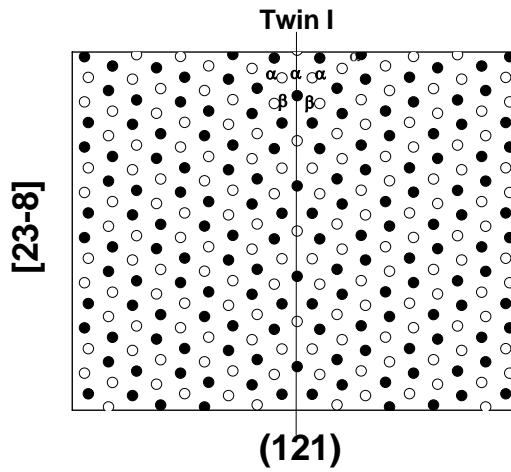Twin I – αβ α βα
Twin II – αβ αβα βα
Twin III – αβ βα

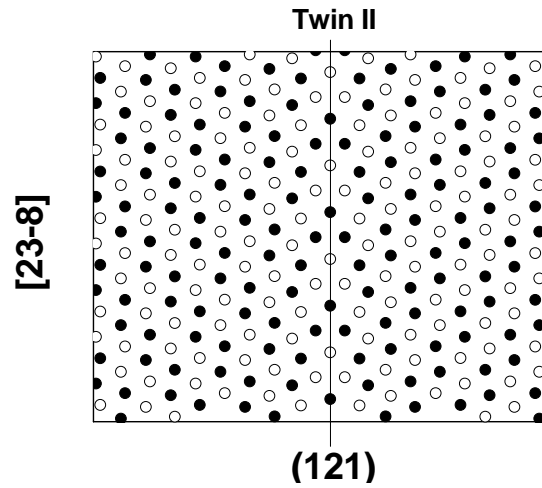**Fig. 5** *Fully relaxed structure of Twin I. The same notation as in Fig. 3.*

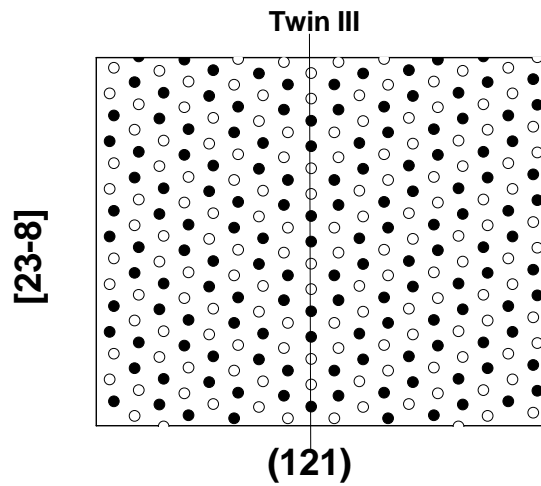**Fig. 6** *Fully relaxed structure of Twin II. The same notation as in Fig. 3.*

Fig. 7 *Fully relaxed structure of Twin III. The same notation as in Fig. 3.*

The results of twin boundaries calculation are listed in Table 3. Twin I possesses the smallest energy among unrelaxed structures but after full relaxations Twin III becomes the structure with the lowest energy. The energy of fully relaxed Twin III structure is about ten times smaller than the energy of Twin I and Twin II structures. The fully relaxed interfaces are shown in Fig. 5-7. The high energy Twin I and Twin II structures were described in [15, 16] as interfaces with row of vacancies in the interface or in the planes neighbour to the interface. Vacancies correspond to the missed α or β subplane of the corrugated $\alpha\beta$ plane. The configuration with uncorrugated central plane was observed experimentally [8] in Cu-Al-Zn alloy. This structure corresponds to the Twin III (Fig. 7).

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Table 3 Energies of unrelaxed and relaxed {121} twin boundaries for p9q1, p9q1.5 and p9q2 potentials. All values are in eV/Å²

		p9q1	p9q1.5	p9q2
Twin I	unrelaxed	0.07823704	0.04539011	0.06129964
	perp. relaxed	0.05534577	0.04205263	0.04699780
	full relaxed	0.03313514	0.03100743	0.02766049
Twin II	unrelaxed	4.35527692	6.480861	8.555070685
	perp. relaxed	0.07705652	0.06066846	0.06476329
	full relaxed	--bcc--	0.04213903	0.030056409
Twin III	unrelaxed	0.09405239	0.06866504	0.09739156
	perp. relaxed	0.0610626	0.04479348	0.04877207
	full relaxed	0.00543276	0.00479014	0.00373147

DISCUSSION

The 2H structure is orthorhombic but it can be recognized as hexagonal if ordering is disregarded in binary and ternary alloys. The results of our calculation are similar to those obtained by Bacon and Liang [17] for the hcp structure and a set of pair-wise potentials. They found that two faults exist on the $\{10\bar{1}1\}$ hcp planes but their positions are potential dependent.

Similar structures for the $\{10\bar{1}1\}$ boundary in the hcp structure were obtained in the calculations by Serra et al. [16]. It was found that low energy boundary has uncorrugated central plane. Two other stable configurations of $\{10\bar{1}1\}$ boundary were found in these calculations, too. They have higher energy than the structure with coalesced planes. These structures are characterized by rows of vacancies either in the interface, or in a plane adjacent to interface.

Thus it is possible to conclude that structure of low energy type I twin boundary is independent on used interatomic potential. The existence of stacking fault in {121} orthorhombic plane is independent on potential as well. But positions of such stacking faults are potential dependent.

The tendency to form uncorrugated planes near the boundary by coalescence of two planes (α and β in Fig. 5) with small interplanar distance is interesting feature. The existence of this tendency allows us to do an assumption about structure of type-II twin boundaries in Cu-Al-Ni 2H martensite. It is known that type-II twins are observed very often in this material. On the other hand as far as we know there are no works which study structure of these boundaries on atomic level. The type-II twin boundaries in the Cu-Al-Ni are observed in irrational plane close to {231}. We can assume that, from physical point of view, irrational boundary is closely approximated by twin in {231} rational plane. Type-II twinning operations are rotation by π around shear direction η_1 or reflection in the plane perpendicular to η_1 [18]. But these twinning operations are not operations of symmetry for {231} plane in 2H structure and thus {231} planes do not coincide in two crystals with twin orientation. The central plane of twin boundaries belong to both twin crystals as a rule. This fact allows to form twin boundary with extremely low energy. Since {231} planes in both twin crystals do not coincide, the formation of low energy twin boundary is possible only if we suppose that central plane in {231} type-II twin consist of two coalesced planes in the similar way as it happens in {121} type-I twin. Such central plane is invariant in respect to twinning operations and can be built into structures of both twin crystals.

CONCLUSIONS

Structure of low energy {121} type-I twin boundary is independent on used interatomic potential. The low energy structure of {121} twin boundary possesses uncorrugated central plane. The existence of stacking fault in {121} orthorhombic plane is independent on potential as well. But positions of such stacking faults are potential dependent.

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