ENERGETICAL PROFILE OF THE SHEAR IN THE ALLOYS WITH THE SUPERSTRUCTURE $D0_{19}$

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Ti_3Al and Mg_3Cd alloys with $D0_{19}$ superstructure on the basis of HCP have many original properties, that is why the research of this systems is very important. In this paper, the method of γ - profile construction is used for the investigation of the crystal state near the planar defect. Stable fault defect, antiphase boundary and complex fault defect, formed in the basis planes {0001}, are obtained. The antiphase boundaries with low level of energy are stable in the prismatic planes $\{10\bar{1}0\}$ and $\{11\bar{2}0\}$. One possible dislocation reaction can take place in Mg_3Cd and Ti_3Al in the basis plane (0001).

1. Introduction

Planar defects, existing in real crystals, are the obstacles for the moving of dislocations. Studying the pictures of atomic displacements in defect areas by the method of computer simulation and calculating the energies of defect formation, we deepen the understanding of the processes, taking place in deformed materials. It is necessary because the mobility of dislocations is determined by the energy of the formation planar defect, connected with the given dislocation. In the ordered alloys, additional effect of strengthening appears at the expense of specific defect, called antiphase boundary (APB).

The detailed analysis of the defect properties and their complexes in the alloys and intermetallids on the basis of BCC and FCC lattices is given in the papers [1,2,3,4,5]. Little attention has been paid to the research of defect complexes in materials on the basis of HCP lattice, though ordered HCP alloys and intermetallids are perspective for the usage in modern technique. The search of stable configurations of planar defects in the ordered Mg_3Cd alloy and Ti_3Al intermetallid is held in the present work.

2. Model description

The stoichiometric composition of $D0_{19}$ superstructure is given by the formation of A_3B. The atoms of both types are situated in the knots of HCP lattice. The configuration of the basis plane (0001) is shown in Fig. 1. The atoms of the "upper" plane are marked by the circles of bigger sizes, the atoms of the "low" plane – by the circles of less sizes. The direction of advantageous shear, forming the planar defect in the basis planes, are $< 12\bar{3}0 >$, in the prismatic planes - $< 2\bar{2}03 >$ and $< 1\bar{2}10 >$.

For the construction of γ - profile, it is made the modelling block of the crystal, containing 120 planes of the given orientation, where the start configuration of the defect is given at the definite vector by the shear of one part of the block relatively to the other. The edges of the crystal block are fastened, and the crystal is allowed to relax till reaching the energetical minimum. The search of the stable configurations of the planar defects is held by the series of the consequence of the bicrystal parts displacements in the chosen difference of the internal energy of the crystal with the defect in the relaxed state and the energy of the ideal crystal.

Internal interactions in the investigating materials are given with the help of anisotropic interatomic potentials of a view:

$$(r,и) = D \cdot в \cdot e^{-бr}(вe^{-бr} - 2) \cdot (1 + o\cos^2 и), \quad (1)$$

where r – the distance between the atoms, θ - the angle between r and the main axis of the crystal. The parameters ξ, α, β, *D* are defined from the stability of the crystal lattices of pure metals (Ti, Al, Mg, Cd) and alloys (Ti_3Al, Mg_3Cd).

3. The results and their discussion

The profiles of γ- surfaces for the Ti_3Al and Mg_3Cd alloys are shown in Figures 2,3,4. γ-surface presents the dependence of the formation energy of the planar defects on the value and the direction of the shear of crystal parts in the definite system of slipping. The

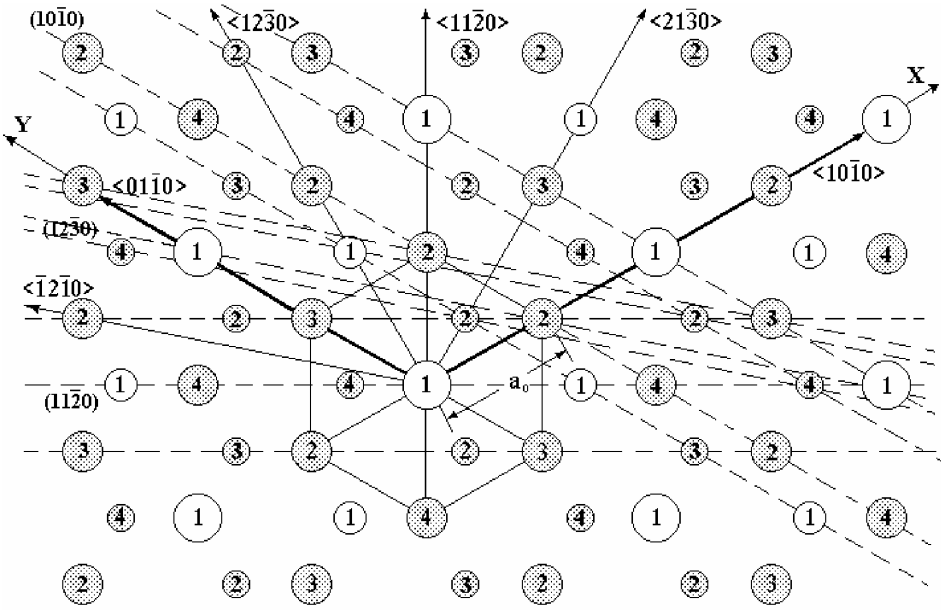

Fig. 1. The projection of the superstructure $D0_{19}$ on the plane (0001). The sublattice numbers are marked 1, 2, 3, 4, correspondingly. The directions of $< 01\ \bar{1}\ 0 >$ and $< 10\ \bar{1}\ 0 >$ types along X and Y coordinate axises are shown by the thick lines. The other crystallographic directions are shown by the thin lines. The steps of the prismatic planes are shown by the dot lines

values of defect formation energy in the start configuration

are shown by the thin line in the pictures and it's equilibrium state – by the thick line.

The minimums at γ- profiles correspond to the stable configurations of the defects. It is worse to note, that all the profiles of γ- surfaces for HCP-system of Ti_3Al correspond to bigger energetical values of the defects formation, than in the system Mg_3Cd. It can be noted, investigating the height of γ- profile height. This phenomena is explained by the fact, that Ti_3Al is an intermetallid and it saves the ordered location

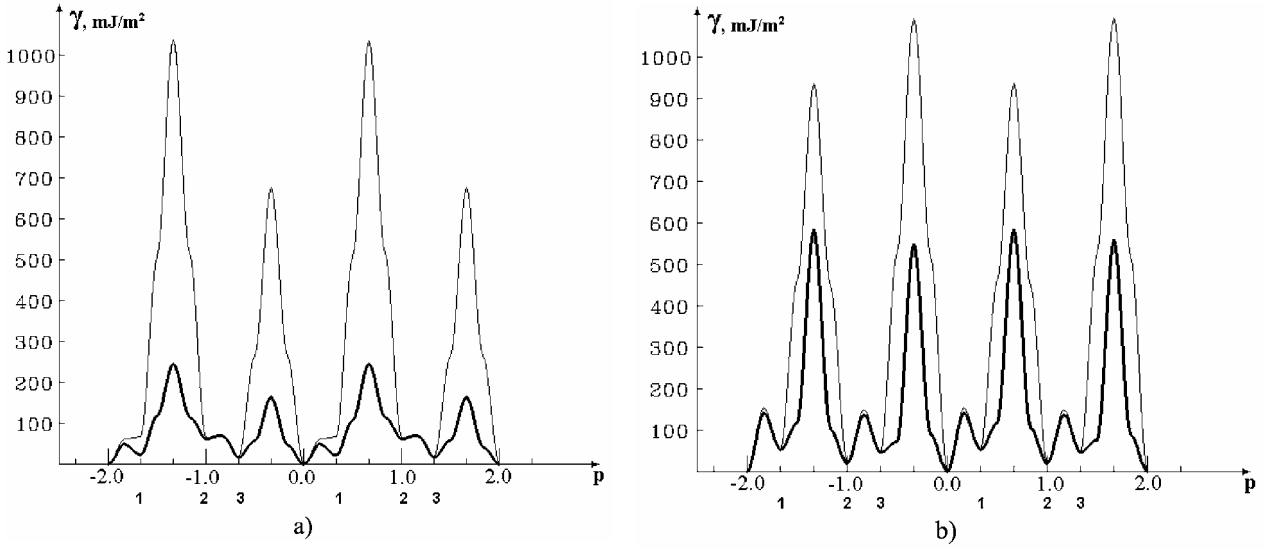

Fig. 2. The dependencies of γ - profiles on the value of the shear vector $\vec{p} = a_0 < 12\bar{3}0 >$ (0001) in the alloy: a) Mg_3Cd, b) Ti_3Al

of the atoms till the melting temperature. There

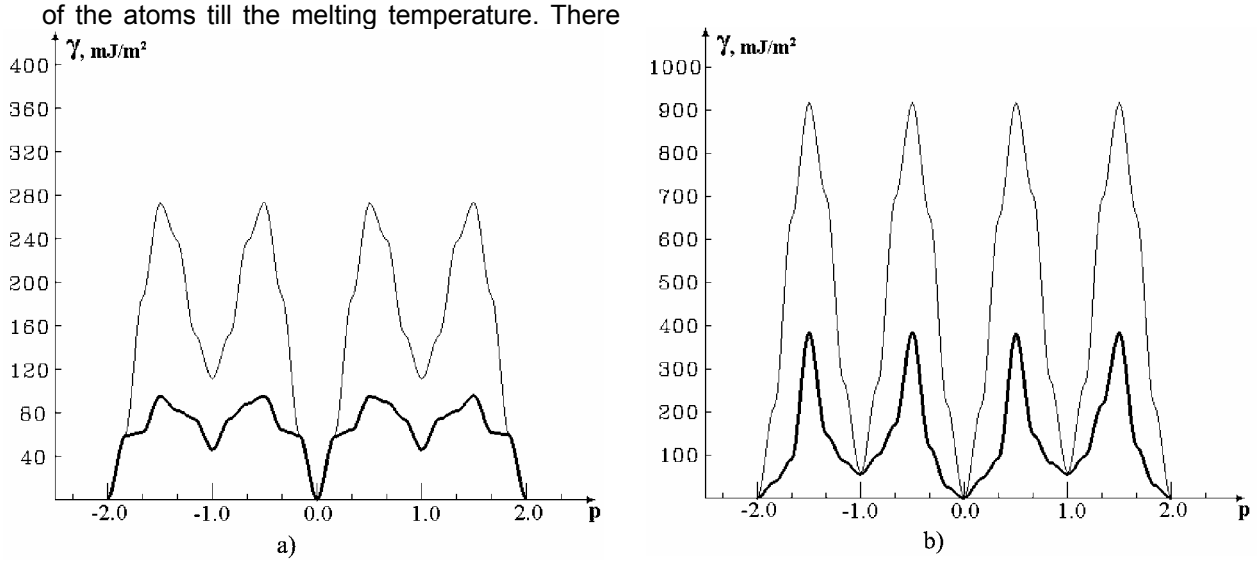

Fig. 3. The dependencies of γ - profiles on the value of the shear vector $\vec{p} = a_0 < 01\,\bar{1}\,0 > (10\,\bar{1}\,0)$ in the alloy: a) Mg_3Cd, b) Ti_3Al

minimums (Fig. 2) at γ- profiles in the basis planes {0001}, which correspond to the fault defect (FD) – the first minimum, APB – the second minimum, the complex fault defect (CFD) – the third minimum. CFD can be considered as a result of applying of FD and APB against each other. It can not be said about γ - surfaces in the planes of the prism $\{10\,\bar{1}\,0\}$ and $\{11\bar{2}0\}$, which profiles are smooth (Fig. 3,4). Only one energetical minimum, corresponding to the stable configuration of APB is well expressed. Energetical values of APB formation in the planes $\{10\,\bar{1}\,0\}$ are bigger (~50 mJ/m^2) than the

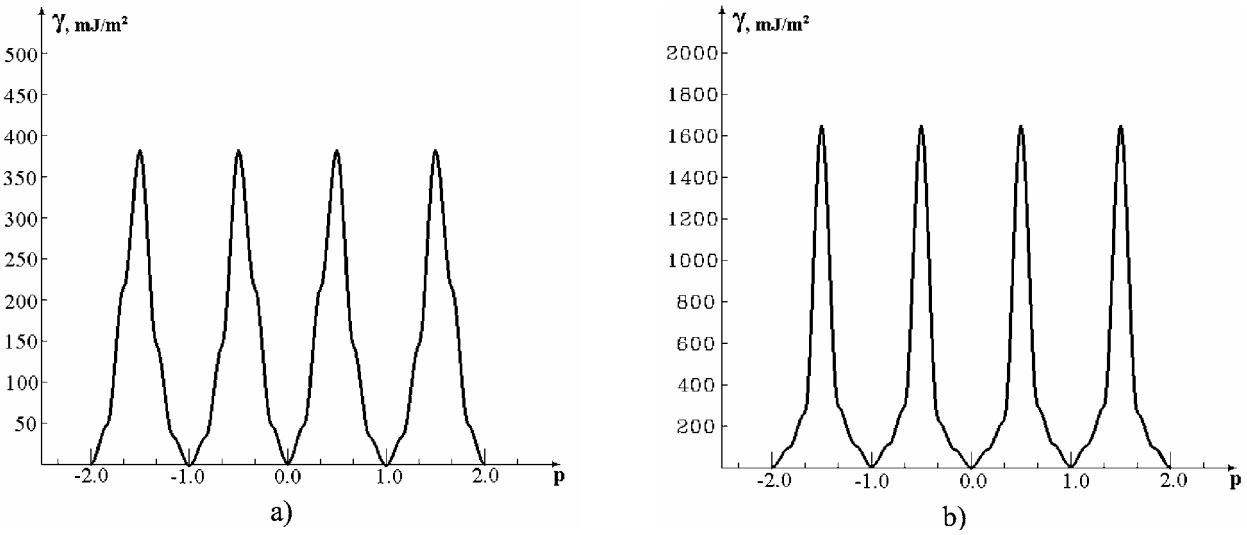

Fig. 4. The dependencies of γ - profiles on the value of the shear vector $\vec{p} = a_0 < 12\bar{3}0 > (11\bar{2}0)$ alloy: a) Mg_3Cd, b) Ti_3Al

energies of APB formation in the planes $\{11\bar{2}0\}$, which are equal to2 mJ/m^2 (for Mg_3Cd alloy) and 4 mJ/m^2 (for the Ti_3Al intermetallid). The start profiles of γ-surfaces of the materials in the prismatic planes $\{11\bar{2}0\}$ are not shown in Fig.4, because they are characterised by very big energetical levels. γ-profiles have well expressed structure, looking like a pike. Consequently, the dislocation reactions in the given group of the planes are absent, because the moving dislocation must pass the essential energetical barriers (~480 mJ/m^2 - for Mg_3Cd and 1600 mJ/m^2 - for Ti_3Al). There are also no dislocation reactions in the planes of the prism, because the value of the shear vector, forming γ- profile, is less than the width of the energetical barrier. One possible dislocation reaction can take place in Mg_3Cd and Ti_3Al in the basis plane (0001) according the following scheme:

$$\frac{a_o}{3}<12\bar{3}0>\leftrightarrow a_o<12\bar{3}0>+\frac{2a_o}{3}<\bar{1}\bar{2}30>. \quad (2)$$

All the formation energies of planar defects, received in the result of the construction and research of γ - profiles, are in satisfactory agreement with the experimental data [6,7,8,9], concerning the Mg_3Cd and Ti_3Al alloys.

4. Conclusion

It is calculated the energetical γ - profiles in Ti_3Al and Mg_3Cd alloys with the superstructure $D0_{19}$. The obtained results prove, that the directions of the advantageous shear, forming the planar defect in the basis planes, are $<12\bar{3}0>$, in the prismatic planes are $<2\bar{2}03>$ and $<1\bar{2}10>$ in these alloys. The stable configurations of the FD, APB, CFD are formed by the vectors of $\pm a_0/3<12\bar{3}0>$, $\pm a_0<12\bar{3}0>$ and $\pm 4a_0/3<12\bar{3}0>$ types, correspondingly, in the basis planes. APB $\pm a_0<2\bar{2}03>\{11\bar{2}0\}$ and APB $\pm a_0<1\bar{2}10>\{12\bar{3}0\}$ can form in the prismatic planes. The discovered stable configurations of the planar defects are the obstacles for the moving of the dislocations. It leads to the deformational strengthening of the studying materials.

REFERENCES

1. Beauchamp P., Dirras G., Phil. Mag. A. 1993. v. 67. № 4. p. 813-826.
2. Mayer J., Elasser C., Fahnel M., Phys. Stat. Sol. B. 1995. 1911 № 2. p. 283-298.
3. Yamaguchi M., Paidar V., Pope D.P., Vitek V., Phil. Mag. A. v. 45. 1982. p. 867.
4. Girifalco L.A., Weizer V.G., Phys. Rev. 1959. v. 114. p. 687-698.
5. Paidar V., Elsevier. 1984. 463 p.
6. MinonishiY., Yoo M.H., Phil. Mag. Lett. 1990. 61. p. 203-208.
7. Umakoshi Y., Nakano T., Sumimoto K., Takenaka T., Yamane T., Acta Met. Mater. 1993. 41. № 4. p. 1149-1154.
8. MinonishiY., Phil. Mag. 1991. 63A. p. 1085-1093.
9. Minonishi Y., Otsuka M., Tanaka H., Japan Inst. of Metals. Sendai. 1991. p. 543-546.

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