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What Types of Stacking Faults and Dislocation Dissociations Can Be Found in Transition-Metal Disilicides

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Identical atomic planes of transition-metal disilicides can form different stacking when they are ordered in several combinations of four different positions A, B, C, D. The following arrangements can be formed: AB in $C11_b$ structure of e.g. $MoSi_2$, ABC in C40 structure of e.g. VSi_2 and ABDC in C54 structure of e.g. $TiSi_2$ disilicides. The ABC atomic plane stacking along the $\langle 111\rangle$ cubic directions is well known in the fcc lattice, where three basic types of stacking faults are known: intrinsic or extrinsic faults and elementary twin, however, other types of stacking faults can be detected in transition-metal disilicides due to the occurrence of the fourth position D. On the other hand, the faults well known in metallic systems as antiphase boundaries need not be metastable in disilicides. Based on the results of *ab initio* calculations, it can be predicted which types of planar defects are metastable corresponding to the local minima on the energy surface of generalized stacking faults or unstable when they are represented, for example, by saddle points. The character of dissociation of the dislocation cores is directly related to the existence of metastable stacking faults. Moreover, the space distribution of dislocation cores has a direct impact on dislocation mobility and, therefore, also on macroscopic mechanical properties of materials. The behaviour of extended crystal defects in disilicides that is caused by covalent interatomic bonding, is discussed starting from the geometrical analysis, and it is demonstrated that predictions of materials properties can be deduced.

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1. Introduction

Transition-metal disilicides ($TMSi_2$) are attractive as structural materials for ultrahigh temperature applications [1, 2]. The crystal structure of these materials is composed of pseudohexagonal atomic planes where all the centres of metallic triangles are occupied by silicon atoms and thus the number of silicon atoms doubles the number of metallic atoms giving the 1:2 stoichiometry ($TMSi_2$). The metallic atoms of neighbouring atomic planes are not situated above the centres of triangles as in metallic structures but bisect the triangle sides. Hence there are four different positions of pseudohexagonal atomic planes, the triangle vertex in a selected reference plane and three centres of triangle sides. In this way the transition-metal disilicides are different from the close-packed metallic structures where the atomic planes with the largest atomic density (the {111} fcc or {0001} hcp planes) can occupy only three different positions (the vertex of a reference triangle and two alternating triangle centres on the plane with hexagonal symmetry). Consequently, three types of structures are generated by different stacking of pseudohexagonal atomic planes in transition-metal disilicides: AB stacking of $C11_b$ structure, ABC stacking of C40 structure and ABDC stacking of C54 structure [3, 4]. The AB stacking is analogous to the hcp metallic structures and the ABC stacking to the fcc structures. Obviously, due to the nature of silicon atoms, the properties and behaviour of transition-metal disilicides are markedly different from the metallic systems.

The stacking faults, in particular their displacement vectors, and related partial dislocations on the basal planes in different types of disilicides will be examined starting from the geometrical analysis that is described in detail in [5]. Subsequently, the related twin boundaries and dissociated dislocations will be discussed. The results and predictions reported here are based on the *ab initio* calculations of so called γ-surfaces (for more details see [6, 7] and our preliminary findings published already in [8]).

2. Stacking-fault-like defects in $C11_b$ structure

The γ-surface is a plot of the energy of generalized stacking faults formed by arbitrary displacements of one crystal half with respect to the other half on a selected crystallographic plane. Relaxations perpendicular to the fault have to be allowed but no relaxations parallel to the fault are permitted. Obviously, such plots preserve the

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periodicity of the selected crystal plane of the hypothetical cut.

The fault energies were calculated in [8] using the pseudopotential method based on the density functional theory as implemented in the Vienna Ab-initio Simulation Package (VASP) code. Only the rigid shift of the crystal parts in a direction parallel to the plane of the stacking fault was allowed. Besides the absolute minima of the perfect crystal (PC), there are local minima of metastable stacking faults (SF) that have the same energies in the $C11_b$ lattice. The displacement to the sites of silicon atoms correspond to the antiphase boundaries (APB) common in metallic systems but such defects are not occurring in disilicides with covalent bonding due to silicon atoms. As it has been shown in [8], there are APB saddle points on the $\{110)$ γ-surface in the case of $MoSi_2$. In the $C11_b$ tetragonal structure, the $\{110)$ plane has the pseudohexagonal symmetry for the c/a ratio of $\sqrt{6}$. The value for $MoSi_2$ is close to it ($c/a = 2.4473$ [4]). Each absolute minimum PC is surrounded by four maxima in the [001] and [110] directions while the local minima of SF lie also between the maxima but in the inclined directions. In addition to the APB saddle points between the maxima in the [001] direction, there are other saddle points between the pairs of two minima and two maxima not marked in Fig. 1.

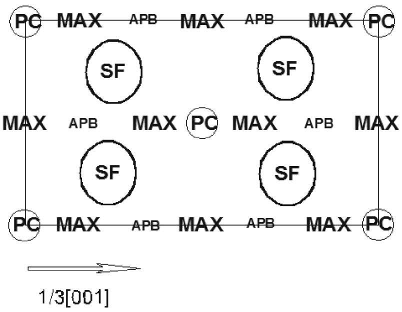

Fig. 1. Geometrical simplification of the γ-surface for $C11_b$ on the $\{110)$ plane. PC indicates the displacements restoring the perfect crystal structure, SF are displacements corresponding to the metastable stacking faults and APB marks the displacements that may form stacking-fault-like defects for metallic bonding. MAX corresponds to the displacements to the unstable atomic configurations.

A hexagon is formed around PC by four local minima SF and two maxima. The $\frac{1}{2}$ [110] displacements PC-MAX has similar magnitude as the $\frac{1}{4}$ [111] displacement PC-SF. However, in the perfect stacking of AB, the PC-SF displacements create AB|DC or AB|CD metastable SF defects while the displacement in the third hexagonal direction would form an unstable AB|BA defect.

3. Stacking-fault-like defects in C40 structure

A larger variety of displacive planar defects can occur in the C40 lattice with the ABC regular stacking. Similarly to the geometrical construction presented in Fig. 1 for the $C11_b$ tetragonal lattice, a schematic γ-surface for the C40 structure on the exactly hexagonal (0001) plane is displayed in Fig. 2. Each absolute minimum PC is surrounded by six APB sites of silicon atoms, however, the local minima denoted as SF between the APB points are not equivalent in the C40 lattice, contrary to the $C11_b$ lattice, as shown in [5]. Again there are four local minima and two maxima around the absolute minimum PC but only the antiparallel PC–SF displacements are equivalent.

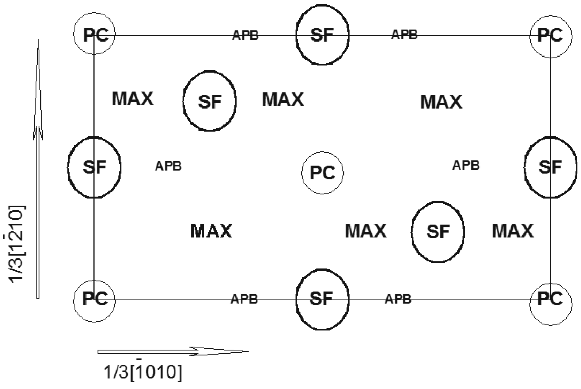

Fig. 2. Geometrical simplification of the γ-surface for the C40 structure on the (0001) plane. Similar notation as in Fig. 1 is employed.

Similarly to the fcc lattice with the ABC stacking, three types of basic stacking faults can be imagined in the C40 lattice: the intrinsic stacking fault ABC|BCA, where the atomic plane in the position A is removed, the extrinsic stacking fault ABC|B|ABC, where the atomic plane in the position B is added, and the elementary twin ABC|B|A|CAB. Let us distinguish two types of planar configurations according to the upper and lower neighbouring atomic planes. The $C11_b$ type plane is BAB or CAC or DAD with the identical upper and lower planes, and the C40 type plane CAB or CAD or BAD with different upper and lower planes. The planes of $C11_b$ type can be considered as incorrect in the C40 stacking. There are two such planes in all three types of basic stacking faults listed above. Hence the twin boundary AB $<$ C $>$ BA, localized on the C plane, contains only one plane of $C11_b$ type having thus roughly about a half energy of the stacking faults. The $<$ C $>$ notation denotes the atomic plane with respect to which the plane stacking is symmetrically ordered. However, the simplest displacive stacking faults in C40 are ABC|BAD or ABC|DCB, when the plane A is shifted to the position B or D, with only one incorrect atomic plane.

4. Stacking-fault-like defects in C54 structure

An analogous approach can be applied to the orthorhombic lattice C54 as well. The basal plane (001) is hexagonal for $a/b = \sqrt{3}$ which is nearly the case for $TiSi_2$ [4] ($a/b = 1.7224$). The schematic γ-surface for the C54 structure on the (001) plane in Fig. 3 is similar to that in Fig. 2. In fact, all three schematic γ-surfaces are similar when the γ-surface for $C11_b$ in Fig. 1 is rotated by 60°.

Also in C54, the SF energies are different since the displacements $\frac{1}{2}$ [010] and $\frac{1}{4}$ [110] are not equivalent. According to our preliminary results, the difference can be very high.

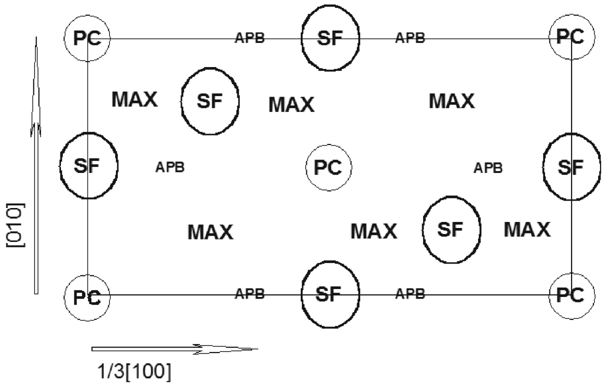

Fig. 3. Geometrical simplification of the γ-surface for the C54 structure on the (001) plane. Similar notation as in Fig. 1 is employed.

5. Dislocation dissociations

The shortest lattice vectors in the three discussed structures are similar as the sides of triangles PC–PC–PC on the pseudohexagonal planes with large atomic density, however, due to different crystal symmetries, they have different crystallographic notations: [110] or 1/2 [111] in $C11_b$, 1/3 <1210] in C40 and [010] or 1/2 [110] in C54. These vectors can be considered as the Burgers vectors of undissociated full dislocations (FD). In all three structures, there is an important anisotropy on the pseudohexagonal plane, namely, a SF occurs in the two directions while it is replaced by a maximum of energy in the third PC–PC direction. Therefore, in the two respective directions the full dislocation can be dissociated into two equivalent partial dislocations (PD):

$$\mathrm{FD} = \mathrm{PD} + \mathrm{PD}. \tag{1}$$

In the third direction, the full dislocation can be dissociated into three non-equivalent partials of the same magnitude but different directions, cup-shape dissociation

$$\mathrm{FD} = \mathrm{PD} + 1/2\mathrm{FD} + \mathrm{PD}. \tag{2}$$

The properties of these dislocations depend substantially on the energy relations among the faults involved and on the spacial character of the dislocation cores. Let us note that not only dissociations on the pseudohexagonal planes are important but the other planes as {310} in $C11_b$ can play a critical role as discussed in [9, 10].

6. Conclusions

Planar defects in transition-metal disilicides on the basal pseudohexagonal planes in the $C11_b$, C40, and C54 structures have been examined. Some of these defects are crucial for understanding the displacive processes that are important for dislocation motion, and consequently, for plastic deformation, or also for phase transformations. It has been shown that, contrary to metallic systems, the standard stacking faults of both intrinsic and extrinsic types are not the most stable displacive defects. Other types of planar defect, such as stacking faults ABC|BAD or ABC|DCB in the C40 structure, that are important for dislocation dissociation, have the energy comparable with the twin boundary, namely AB < C > BA.

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