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Planar defects and dislocations in transition-metal disilicides

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ABSTRACT

The structures of transition-metal disilicides are constituted of different stacking of identical atomic planes at four different positions **A**, **B**, **C**, **D**: **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. In comparison with the FCC lattice with the **ABC** atomic plane stacking along the <111> directions, the occurrence of the fourth position, **D**, essentially alters the properties of defects and consequently the mechanical properties. The effect of generalized planar defects and their impacts on the dislocation core structures are discussed. In particular, we examine stacking faults and related partial dislocations on the basal planes in different types of disilicides as well as the related twin boundaries and dissociated dislocations. Our analysis of the stacking-fault-like defects is based on the calculations of γ-surfaces using ab initio methods. Predictions of possible metastable defects in all types of disilicides are reported.

1. Introduction

Transition-metal disilicides have been studied as functional materials with applications in the microelectronics industry [1] as well as perspective structural materials for ultra-high temperature applications [2,3]. Structures of these materials may be considered as composed of pseudohexagonal atomic planes where the centres of metallic triangles are occupied by silicon atoms. Consequently, the metallic atoms of the neighbouring atomic planes are not situated in the centres of triangles, as in the metallic FCC or HCP structures, but bisect the triangle sides as depicted in Fig. 1. In the pseudohexagonal atomic planes, each metallic atom has six silicon nearest neighbours while each silicon atom has three metallic and three silicon nearest neighbours. The metallic atoms of the neighbouring atomic planes are situated above the centres of underlying pairs of silicon atoms and simultaneously above the centres of metallic bonds. Three centres of triangle sides together with the initial position at the triangle apex form four different positions for parallel pseudohexagonal atomic planes as shown in Fig. 1. Three types of structures are generated by different stacking of pseudohexagonal atomic planes: **AB** stacking of $C11_b$ structure, **ABC** stacking of C40 structure and **ABDC** stacking of C54 structure [4,5]. **AB** stacking of close-packed planes is analogous to the HCP metallic structures and **ABC** stacking to the FCC structures. However, due to the positions and bonding of silicon atoms, the properties and behaviour of transition-metal disilicides are markedly different from metallic systems.

Our approach is based on the geometrical analysis of atomic configurations of possible stacking faults. For this purpose, we deal with so-called γ-surfaces. They are defined as the energies of perturbed crystal when one half is displaced with respect to the other half on a chosen crystallographic plane. The energy plot as a function of the displacement vector is named the γ-surface. These energies were calculated for selected disilicides using ab initio methods. Then the topology of such surfaces is generalized for other disilicide systems. Only the most densely packed atomic planes in different crystal structures are considered here. On the basis of examined stacking faults, possible types of partial dislocations are found in different types of disilicides on the respective basal planes. Subsequently, the related twin boundaries and dissociated dislocations are discussed. In this way, the predictions of metastable stacking-fault-like defects and their effect on

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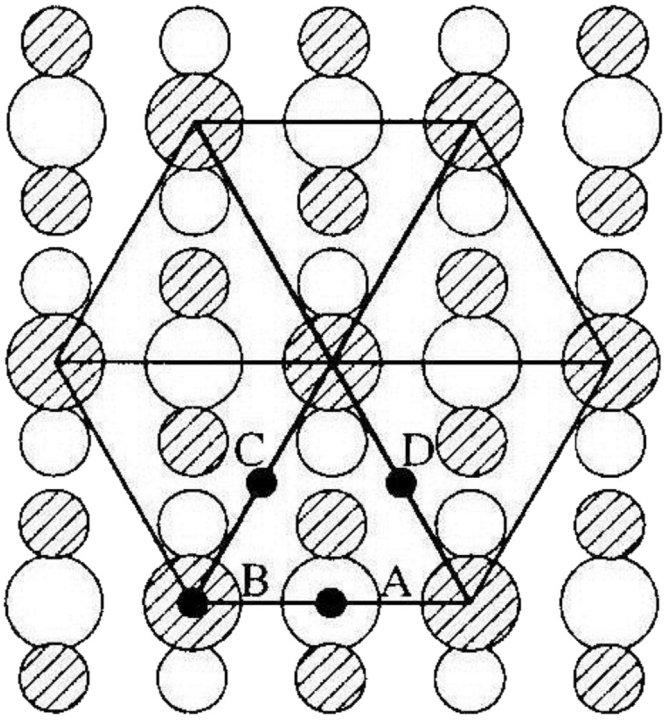

Fig. 1. Hexagonal atomic arrangement in transition-metal disilicides. Large circles represent metallic atoms, small circles silicon atoms, hatching distinguishes two depicted neighbouring atomic layers in the projection direction. Possible positions of metallic atoms in the neighbouring parallel atomic planes are denoted as **A**, **B**, **C**, **D**.

dislocation core structures, and so on dislocation mobility, can be performed.

2. Computational details

Electronic structure of the systems studied here was calculated using the pseudopotential method based on the density functional theory as implemented in the VASP (Vienna Ab-initio Simulation Package) code [6–8]. The electron–ion interactions were treated using projector-augmented wave (PAW) method [9,10] and the exchange-correlation functional was described within the generalized gradient approximation (GGA) [11]. To ensure the reliability of our results we used the energy cut-off for the plane waves of 400 eV and the k-point density of 5000 Å^3. The Brillouin-zone integrations were performed with the help of the tetrahedron method with Blöchl corrections. Full structural relaxation was carried out (i.e. position of the ions, volume and shape of the supercell), All forces were smaller than 0.01 eV/Å.

First we have found the equilibrium structures of VSi_2, $MoSi_2$ and $TiSi_2$. The calculated lattice parameters agree very well (within 0.65%) with the experimental values given in Ref. [5].

When calculating the γ-surfaces, only the rigid shift of the crystal parts in a direction parallel to the plane of the stacking fault was allowed. In VSi_2, the (0001) γ-surface was obtained with the help of the supercell containing 18 atoms distributed in 6 atomic layers. This supercell was created by doubling the original C40 cell (9 atoms, 3 atomic layers) along the *z*-axis. Then, vacuum layer of the same thickness as double C40 cell along the *z*-axis was introduced, i.e. the dimension of the supercell along the *z*-axis amounted to $c_{\text{supercell}} = 4*6.365$ Å $= 25.46$ Å. This approach prevents periodic images of the stacking faults to interact.

The (110) γ-surface in $MoSi_2$ and the (001) γ-surface in $TiSi_2$ were calculated using the supercell with 36 atoms arranged in 6 atomic layers along the [110] axis and the supercell with 24 atoms in 8 atomic layers along the [001] axis, respectively. Then, similarly as in the case of the γ-surface for VSi_2, vacuum layer of the same thickness was added. We have not performed convergence tests w.r.t. number of atomic layers. However, on the basis of our previous experience with grain boundaries, it may be supposed that the periodically arranged stacking faults do not interact or, if so, their interaction may be neglected.

3. Stacking-fault-like defects in C40

Let us start with the displacive defects situated on the hexagonal plane (0001) in the **ABC** regular stacking of the C40 structure. Geometrically possible faults, commonly occurring in metallic systems, are of three types: antiphase boundaries (APB), where the metallic atom is shifted to the position of the other element (here silicon), superlattice stacking faults (SF), when one crystal half is shifted into another position from **A**, **B**, **C**, **D** (see Fig. 1), and complex stacking faults (CSF) (for more details see Ref. [12]). Such defects may appear as local minima on the γ-surface which 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 periodicity of the selected crystal plane of the hypothetical cut. More details on the notion of γ-surfaces can be found in Refs [13–15].

The fault energies must be calculated in a reliable model respecting the character of bonding forces. Due to covalent bonding in silicides, an approach based on the modifications of the electronic structure of the perfect crystal, caused by the defect, must be employed. The γ-surface for the (0001) plane in VSi_2 with C40 structure is plotted in Fig. 2. Let us note that besides the absolute minima corresponding to the perfect crystal, there are local minima of metastable stacking faults, in fact of two types but with similar energies (0.435 and 0.447 J/m^2).

The actual positions of local minima can be compared with the geometrically possible faults derived without specification of the material type, based only on the symmetry of the particular crystal lattice. Such a γ-surface for the C40 lattice is schematically shown in Fig. 3. Only the superlattice stacking fault type defects (SF) correspond to the local minima of metastable faults on the γ-surfaces for VSi_2. The graphical presentation of the energies of generalized stacking faults as the function of displacement vector indicates the energies as well as the displacement vectors of

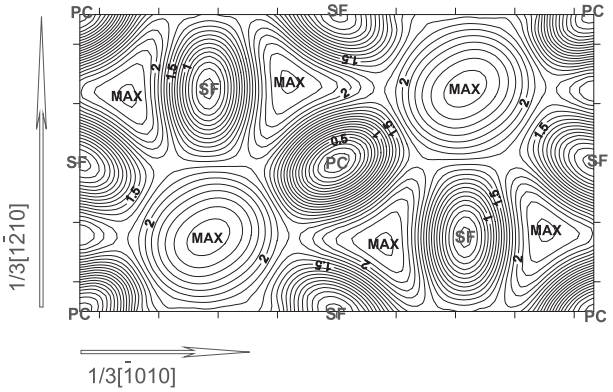

Fig. 2. Ab initio calculated γ-surface for VSi_2 with the C40 structure on the (0001) plane. PC indicates the absolute minima of the perfect crystal, SF are metastable minima of stacking faults and MAX are local maxima points of two types. The energies of generalized stacking faults are expressed in J/m^2 marked on the contour lines.