Theoretical analysis of dislocation splittings in MoSi$_2$

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Abstract. Due to a lower symmetry of the tetragonal C11b structure when compared with the cubic BCC lattice, the $1/2<331>$ dislocation cores are split asymmetrically contrary to the $1/2<111>$ BCC dislocations. This has essential impact on their behaviour and, consequently, on mechanical properties. Various types of dislocation dissociations are analyzed in the frame of anisotropic elasticity with the help of the data from ab initio calculations of $\gamma$-surfaces for generalized stacking faults.

1. Introduction

The intermetallic compound MoSi$_2$ crystallizes in the body-centred-tetragonal C11b structure. The C11b lattice of this binary system is similar to the BCC lattice but the dimension $c$ in the tetragonal direction is not $3a$ but is close to $a\sqrt{6}$ [1]. The bonds between all nearest Mo and Si atoms have the same length for the ideal $c/a$ ratio equal to $\sqrt{6}$ and internal structure parameter $\Delta = 0$ [1]. Various slip systems can be activated in MoSi$_2$ for different sample orientations and temperatures [2-10] but for the compressive deformation along the tetragonal axis <001>, the plastic deformation is exclusively controlled by the mobility of the $1/2<331>$ dislocations on the {013} planes. These dislocations are important for ductility of molybdenum disilicide in general and this is why they deserve a special attention. The $1/2<331>$ dislocations are in fact inherited from the $1/2<111>$ dislocations of the BCC crystals. Orientation dependence of the critical resolved shear stress clearly indicates that the dislocation properties of $1/2<331>$ dislocations are governed by their cores.

The first step in the dislocation core structure examination is determination of the existence of stacking faults and related calculations of the energies of generalized stacking faults. These planar defects are decisive for the dislocation core structure and their properties can be assessed using a suitable model of interatomic forces. Due to a rather complex interatomic bonding in silicides, a quantum-mechanical density functional based ab initio method was employed in the calculations of $\gamma$-surfaces, i.e. the energies of generalized stacking faults as functions of displacement vectors [11] that answers the above question.
Here we report the first results of our theoretical study. Our analysis of possible dislocation splittings utilizes anisotropic linear elasticity and is based on the \textit{ab initio} calculations of the $\gamma$-surface.

2. Dissociations of the 1/2\bs{331} screw dislocations

Due to a long 1/2\bs{331} Burgers vector, the dislocation energy is high, and therefore, the activity of such dislocations with this Burgers vector is rather unexpected. Nevertheless, the most important factor is dislocation mobility that can be enhanced by appropriate dislocation dissociation.

Let us start with the planar dislocation splittings on the (013) plane that is related to the (011) BCC plane with large atomic density. There are three local minima on the $\gamma$-surface corresponding to three different non-crystallographic stacking faults (SF) on the (013) plane [11]. The vectors connecting these minima with the deepest minimum corresponding to the ideal crystal (IC) are possible Burgers vectors of partial dislocations. Three dislocation reactions with the Burgers vectors of partials that deviate least from the $[\overline{3}31]$ direction are

\begin{align}
    \vec{b} &= \vec{b}_1 - \text{SF2} - \vec{b}_2, \\
    \vec{b} &= \vec{b}_3 - \text{SF1} - \vec{b}_4 - \text{SF3} - \vec{b}_5, \\
    \vec{b} &= \vec{b}_3 - \text{SF1} - \vec{b}_6 - \text{SF2} - \vec{b}_7 - \text{SF3} - \vec{b}_5.
\end{align}

The Burgers vectors $\vec{b}_1$ to $\vec{b}_7$ are defined in tables 1-3 and marked in figure 1 on the contour plot of the (013) $\gamma$-surface.

![Figure 1. Contour plot of the (013) $\gamma$-surface and dissociations of the 1/2 $[\overline{3}31]$ dislocation on the (013) plane. Three types of dissociations are depicted: Twofold $\vec{b}_1+\vec{b}_2$, threefold $\vec{b}_3+\vec{b}_4+\vec{b}_5$ and fourfold $\vec{b}_3+\vec{b}_6+\vec{b}_7+\vec{b}_5$ dissociations. Minima of the $\gamma$-surface corresponding to the non-perturbed ideal crystal are marked as IC and the positions of three stacking faults as SF1, SF2 and SF3.](image)

| Burgers vector dissociation | $\vec{b}_1$ | $\vec{b}_2$ |
|----------------------------|------------|------------|
| $\gamma$-surface minima     | IC-SF2     | SF2-IC     |
| angle to $[\overline{3}31]$ | 14.5°      | 14.5°      |
Table 2. Threefold planar dissociation of the 1/2 [3 3 1] dislocation on (013).

| Burgers vector | b3 | b4 | b5 |
|----------------|----|----|----|
| γ-surface minima | IC-SF1 | SF1-SF3 | SF3-IC |
| angle to [3 3 1] | 9.3° | 12.6° | 14.5° |

Table 3. Fourfold planar dissociation of the 1/2 [3 3 1] dislocation on (013).

| Burgers vector | b3 | b6 | b7 | b5 |
|----------------|----|----|----|----|
| γ-surface minima | IC-SF1 | SF1-SF2 | SF2-SF3 | SF3-IC |
| angle to [3 3 1] | 9.3° | 37.8° | 14.5° | 14.5° |

The dissociation widths can be determined from the equations for the balance between the surface tensions of stacking faults and the dislocation interaction forces. In the framework of anisotropic elasticity, these forces depend on the orientation of dislocation line, the Burgers vectors and the elastic constants [12]. For the twofold dissociation, the width $r_1$ of stacking fault ribbon is given by

$$\gamma_2 = F12/r_1,$$

(4)

where $F12$ is the force parameter between the partials and $\gamma_2$ is the stacking fault energy.

For the threefold dissociation, two widths $r_2$ and $r_3$ are given by

$$\gamma_1 = F34/r_2 + F35/(r_2+r_3),$$

(5)

$$\gamma_3 = F54/r_3 + F53/(r_2+r_3),$$

(6)

$$F43/r_2 + \gamma_3 = F45/r_3 + \gamma_1.$$  

(7)

And finally, for the fourfold dissociation, three widths $r_4$, $r_5$ and $r_6$ are given by

$$\gamma_1 = F36/r_4 + F37/(r_4+r_5) + F35/(r_4+r_5+r_6),$$

(8)

$$\gamma_3 = F57/r_6 + F56/(r_5+r_6) + F53/(r_4+r_5+r_6),$$

(9)

$$F63/r_4 + \gamma_2 = F67/r_5 + F65/(r_5+r_6) + \gamma_1,$$

(10)

$$F75/r_6 + \gamma_2 = F76/r_5 + F73/(r_4+r_5) + \gamma_3.$$  

(11)

The single-crystal elastic constants of tetragonal MoSi$_2$ corresponding to the temperature of 0 K were taken from [13] (c11=410 GPa, c33=514 GPa, c12=115 GPa, c13=87.5 GPa, c44=207 GPa and c66=200 GPa) and the c/a ratio of 2.447 ($a = 0.3206$ nm, $c = 0.7846$ nm) was used in the calculations of the force parameters $F_{ik}$ for dislocation interaction forces $F_{ik}/r$ where $i$ and $k$ denotes different pairs of partial dislocations. The energies of three stacking faults on the (013) plane determined by $ab$ initio calculations are $\gamma_1 = 1.22$ J/m$^2$, $\gamma_2 = 1.06$ J/m$^2$, and $\gamma_3 = 1.12$ J/m$^2$ [11].

The separation $r_1$ of the $b_1$ and $b_2$ partials that divide the total Burgers vector into two parts was found to be about 12a. The threefold dissociation $b_3+b_4+b_5$ is slightly wider, both separations $r_2$ and $r_3$ are about 7a. Finally, the widths $r_4$, $r_5$ and $r_6$ of the stacking fault ribbons for the fourfold dissociation $b_3+b_6+b_7+b_5$ are 4a, 7a and 5a, respectively. The partial dislocation separations are expressed in units of the lattice constant $a$ (0.3206 nm) that determines the C11$_b$ lattice dimensions. Dislocation dissociation causes an energy decrease that grows with the number of partial dislocations. For the twofold dissociation the energy gain is about $6.3\times10^{-9}$ Jm$^{-1}$, for the threefold dissociation it is $6.8\times10^{-9}$ Jm$^{-1}$ and for the fourfold dissociation $8.3\times10^{-9}$ Jm$^{-1}$.
The direction of \([3\overline{3}1]\) is parallel to the intersection of three planes with large atomic densities, namely \((013), (\overline{1}03)\) and \((110)\). Those three planes are analogous to the \{110\} planes in the BCC lattice into which the most common BCC Burgers vector \(1/2<111>\) can spread. The calculations of the \(\gamma\)-surface on the \((110)\) plane found that the stacking fault energy on this plane is considerably smaller, \(\gamma_0 = 0.357 \text{ J/m}^2\), than on \((013)\) \cite{11}. The displacement vector is either \(1/4 [3\overline{3}1]\) or \(1/2 [1\overline{1}1]\) leading in both cases to the same crystallographic stacking fault on \((110)\). Nevertheless, the Burgers vector \(1/2 [1\overline{1}1]\) is less likely to participate in the dissociation of \(1/2 [3\overline{3}1]\) since it is inclined by 30° to the \([3\overline{3}1]\) direction, and the corresponding dislocation energy is thus much higher than for the dissociations with \(1/4[3\overline{3}1]\).

Assuming the dissociation \(b/2+b/2\) with the low stacking fault energy \(\gamma_0\) we get the splitting width of about 39a. However, such a dissociation is not possible on the \((013)\) plane as there is no local minimum for the displacement \(1/4 [3\overline{3}1]\). Similarly as in the case of \(1/2<111>\) screw dislocation in a BCC structure, the screw dislocation \(1/2 [3\overline{3}1]\) may dissociate in a non-planar manner on the three planes \((013), (\overline{1}03)\) and \((110)\) with the Burgers vectors \(b3\) and \(b3^*\) on \((013)\) and \((\overline{1}03)\), respectively, together with \(b/2\) on \((110)\). A small Burgers vector \(bc3\) (12.8% of \(b/2\)) will remain in the dislocation centre at the intersection of three planes. An alternative non-planar dissociation is into \(b5\) and \(b5^*\) on \((013)\) and \((\overline{1}03)\), respectively, together with \(b/2\) on \((110)\). The central dislocation \(bc5\) is even slightly smaller (11.5% of \(b/2\)) in this case. The Burgers vectors \(b3^*\) and \(b5^*\) lying on \((\overline{1}03)\) are analogous to the vectors \(b3\) and \(b5\) lying on \((013)\); they have the same lengths but different orientations.

Due to a low value of the energy \(\gamma_0\) the non-planar threefold dissociations are much wider than the planar ones. Neglecting the small central dislocations the separation of the partial \(b/2\) from the central dislocation is about 80a, while the widths of \(\gamma_1\) or \(\gamma_3\) on the \{013\} planes are about 2a in both cases. When the interaction forces with the central dislocation are taken into account the separation of \(b/2\) slightly increases to 82a for the \(b3+b3^*+b/2\) reaction while it remains nearly the same for the \(b5+b5^*+b/2\) reaction. These dislocation splittings practically look as dissociations into two partials with the Burgers vectors \(b/2\) and with the core of the partial at the intersection as spread into the two planes of the \{013\} type. The energy gain is larger for the \(b3\) and \(b3^*\) partials (13.0 \(10^{-9}\) Jm\(^{-1}\)) than for the \(b5\) and \(b5^*\) partials (10.8\(\times\)10\(^{-9}\) Jm\(^{-1}\)). Nevertheless, these energetical gains due to splitting on \((110)\) are larger than those for any planar dissociation \((1), (2)\) or \((3)\).

3. Dissociations of the \(1/2<131>\) screw dislocations

There are other Burgers vectors of the dislocations on the \((013)\) plane that are shorter than \(1/2<331>\). We will not discuss here the dislocations \(<100>\) and \(<110>\) lying on the \((001)\) basal plane as those dislocations are not active for loading along the hard \(<001>\) tetragonal direction. Similarly, the dislocations \(<001>\) and \(1/2<1\overline{1}1>\) on the \((110)\) plane will not be considered for the same reason. Notice that the dislocation \(<001>\) have a comparable length with \(1/2<331>\). Nevertheless, there are also dislocations \(bi = 1/2<131>\) inclined to the direction of \(<331>\) on the \{013\} plane that are shorter than \(b = 1/2<331>\).

Two dislocation reactions with the Burgers vectors close to the \([1\overline{3}1]\) direction can be envisaged:

\[
\begin{align*}
bi &= b1 \quad -SF2- b8, \\
bi &= b3 \quad -SF1- b6 \quad -SF2- b8.
\end{align*}
\]  

These Burgers vectors are defined in tables 4-5 and in figure 2. The dissociation widths can be again determined from the balance between the surface tensions of stacking faults and the dislocation interaction forces. For the twofold dissociation of \(1/2 [1\overline{3}1]\), the width \(r7\) is given by

\[
\gamma_2 = F18/r7.
\]
Figure 2. Dissociations of the 1/2 [1 3 1] dislocation on the (013) plane. Two types of dissociations are depicted: Twofold $b_1 + b_8$ and threefold $b_3 + b_6 + b_8$ dissociations.

Table 4. Twofold planar dissociation of the 1/2 [1 3 1] dislocation on (013).

| Burgers vector | $b_1$ | $b_8$ |
|----------------|-------|-------|
| $\gamma$-surface minima | IC-SF2 | SF2-IC |
| angle to [1 3 1] | 8.8° | 14.5° |

Table 5. Threefold planar dissociation of the 1/2 [1 3 1] dislocation on (013).

| Burgers vector | $b_3$ | $b_6$ | $b_8$ |
|----------------|-------|-------|-------|
| $\gamma$-surface minima | IC-SF1 | SF1-SF2 | SF2-IC |
| angle to [1 3 1] | 32.6° | 14.5° | 14.5° |

Finally, for the threefold dissociation of 1/2 [1 3 1], two widths $r_8$ and $r_9$ are given by

\[
\gamma_1 = F_{36}/r_8 + F_{38}/(r_8+r_9), \tag{15}
\]
\[
\gamma_2 = F_{86}/r_9 + F_{83}/(r_8+r_9), \tag{16}
\]
\[
F_{63}/r_8 + \gamma_2 = F_{68}/r_9 + \gamma_1. \tag{17}
\]

The separation $r_7$ of the $b_1$ and $b_8$ partials that divide the Burgers vector $b_i$ into two parts was found to be about $8a$. The threefold dissociation $b_3 + b_6 + b_8$ is again slightly wider, the separations $r_8$ and $r_9$ are about $3a$ and $7a$, respectively. The energetical gains for these planar dissociations are 3.5 and $4.0 \times 10^{-9}$ J m$^{-1}$, respectively, what is much smaller than for the non-planar dissociations.

4. Discussion

The main difference between the two dislocations $b=1/2<331>$ and $b_i=1/2<131>$ is that the screw dislocation $b_i$ inclined by 23.3° to the [3 3 1] direction cannot spread into the (110) plane and cannot thus profit from the energy decrease due to the low energy stacking fault on (110).
The lengths of all the Burgers vectors $b_3, b_6, b_7, b_5, b_8$ are comparable, the important difference is the deviation of $b_6$ from the $[3\overline{3}1]$ direction and of $b_3$ from the $[1\overline{3}1]$ direction. Due to this deviation the respective dislocation interaction forces are weaker and the splitting $b_3+b_6+b_8$ is asymmetric contrary to the splitting $b_3+b_4+b_5$ that is symmetric (cf. tables 5 and 2, the dissociation widths being 3.1$a$ and 7.3$a$ vs. 7.2$a$ and 7.1$a$). Assuming the same energies of the stacking faults, $\gamma_1 = \gamma_2 = 1.14$ J/m$^2$, the separations $r_8$ and $r_9$ are 3.5$a$ and 6.6$a$, respectively, while for the calculated energies they are 3.1$a$ and 7.3$a$, respectively. It shows that there is certain effect of the stacking fault energy difference but since this difference is relatively small (15%), the deviation of the $b_3$ Burgers vector from the direction of the screw dislocation ($32.6^\circ$) has a more pronounced effect on the asymmetrical character of dissociation.

The reported widths of dislocation splitting are accessible by modern electron microscopes and so it is a challenge for experimentalists to test our theoretical predictions. For this purpose the weak-beam technique is considered to be very promising [14].

Due to the asymmetrical splittings a strong anisotropic behaviour of the $1/2<331>$ dislocations can be expected. There are two non-planar dissociations, $b_3+b_3^*+b/2$ and $b_5+b_5^*+b/2$ that have similar nature and more detailed investigation would be necessary to describe their behaviour. Since the dislocation mobility is of primary importance, the effect of applied stresses has to be considered.

5. Conclusions

In addition to numerous planar dislocation splittings on the \{013\} planes, the non-planar core structures were reported that can play an important role in plastic deformation of C11b disilicides, in particular they may cause strong orientation dependence of mechanical properties of single crystals. This dislocation behaviour is much more complex than that of BCC $1/2<111>$ dislocations.

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