Journal of Alloys and Compounds 632 (2015) 44–47

Contents lists available at ScienceDirect

Journal of Alloys and Compounds

journal homepage: www.elsevier.com/locate/jalcom

Letter

Why the slip of 1/2⟨331] dislocations on {013) in $C11_b$ behaves differently at low and high temperatures?

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ARTICLE INFO

Article history:
Received 17 December 2014
Received in revised form 16 January 2015
Accepted 21 January 2015
Available online 30 January 2015

Keywords:
High-temperature alloys
Intermetallics
Atomic scale structure
Dislocations
Mechanical properties

ABSTRACT

The 1/2⟨331] dislocations in the tetragonal $C11_b$ structure of disilicides may possess a threefold non-planar core structure inherited from the BCC lattice. Due to non-metallic bonding, the dislocation splitting is intrinsically asymmetrical what has large consequences for dislocation properties. The 1/2⟨331] slip on the {013) planes was observed at high temperatures above 900 °C when compressed along [001], but surprisingly, also below 500 °C when compressed along [0151]. Why different dislocation behaviour is observed at high and low temperatures is explained in this paper.

1. Introduction

Transition-metal disilicides have been studied for decades not only as functional materials but also as perspective structural materials for ultra-high temperature applications [1,2]. However, complex dislocation behaviour in these materials has not yet been completely understood. One of fundamental questions is why the slip of dislocations with the large Burgers vectors of 1/2⟨331] on the {013) planes occurs in a completely different way at high and low temperatures.

The crystal structure of the most studied disilicide $MoSi_2$ is $C11_b$ that is a tetragonal structure composed essentially from three BCC type elementary cells – see Fig. 1. For the c/a ratio of $\sqrt{6}$, the atomic arrangement on the (110) plane is pseudohexagonal with sixfold symmetry. Many different slip systems were analysed in $MoSi_2$ [3] including the slip along the ⟨100] short Burgers vector on several crystallographic planes as {010), {011) or {023) and the 1/2⟨111] slip on the {110) plane. For the load direction along the [001] tetragonal axis, the 1/2⟨331] {013) slip is observed only at high temperatures above 900 °C while for the [0151] load direction, the same slip is active at low temperatures below 500 °C. Relatively not too high values of CRSS for the 1/2⟨331] {013) slip were observed at low temperatures, contrary to a steeply increasing CRSS with decreasing temperature that was found at high-temperature zone – see Fig. 2.

The tetragonal $C11_b$ structure would become the BCC lattice if there were not two different species in the unit cell, metallic and silicon atoms. Consequently, there are certain aspects of dislocations in the $C11_b$ compounds that appear to emulate the dislocation properties in BCC metals, nevertheless, due to entirely different atomic bonding in disilicides, in comparison with metallic systems, there are huge differences in dislocation behaviour as discussed below.

2. 1/2⟨331] dislocations

The 1/2⟨331] dislocations are in fact inherited from the 1/2⟨111] dislocations of the BCC crystals. In compression along the [001] $C11_b$ tetragonal axis, the plastic deformation is exclusively controlled by the mobility of 1/2⟨331] dislocations. This is the case in spite of the fact that for the ideal c/a ratio of $C11_b$, the magnitude of the 1/2⟨331] Burgers vector is $\sqrt{6}$ larger than that of the ⟨100] Burgers vector.

The structure of dislocation cores is related to the crystal symmetry of the direction of the dislocation line. An important material characteristic is whether metastable stacking-fault-like defects exist on planes containing the dislocation line. While no such stacking fault is known in BCC metals, metastable faults were found on the {013) and {110) planes in $MoSi_2$ with the $C11_b$ structure by *ab initio* calculations of γ-surface [4]. Using these results,

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http://dx.doi.org/10.1016/j.jallcom.2015.01.154
0925-8388/

the non-planar dissociations of screw 1/2⟨331] dislocations in $MoSi_2$ can be analysed and their impact on dislocations glide can be discussed.

Due to a rather complex interatomic bonding in silicides, a quantum–mechanical density functional based *ab initio* method was employed in the calculations of γ-surfaces, i.e. the energies of generalised stacking faults as functions of displacement vectors [4]. Only one type of the metastable stacking fault can occur on the {110) plane while three different metastable stacking faults were identified on the {013) plane. The energies of these three stacking faults on {013) are relatively high and very similar (1.22, 1.06 and 1.12 J/m^2) while the stacking fault energy on the {110) plane is appreciably lower (0.357 J/m^2). A non-planar threefold dissociation related to the well known dissociation of screw dislocations in BCC crystals can be anticipated – see Fig. 3.

Planar dissociations of the 1/2⟨331] dislocations on the {013) planes had already been discussed in our previous paper [5]. In this paper, we concentrate on possible impacts of dissociations of the 1/2⟨331] dislocations that relate crystallographically to the 1/2⟨111] dislocations in BCC crystals. We focus on non-planar splitting of screw dislocations and discuss an analogy between splitting in $C11_b$ crystals and core spreading in BCC metals. $MoSi_2$ was studied extensively experimentally [2] and it is a system for which the stacking faults were identified in calculations employing a density functional theory (DFT) based method [4]. But our results can be generally valid for other $C11_b$ crystals as well.

3. Slip of 1/2⟨331] dislocations on {013) planes

In BCC metals, the core of the 1/2⟨111] screw dislocation spreads into three {101) planes of the ⟨111] zone. This non-planar core is responsible for a high Peierls stress of screw dislocations, which owing to their low mobility control then the plastic behaviour of BCC metals.

In the $C11_b$ lattice, two {013) planes are equivalent but the third plane from the ⟨331] zone, the {110) plane, is geometrically different. The non-planar splitting of 1/2⟨331] screw dislocations in the $C11_b$ lattice is intrinsically asymmetrical while the core spreading of the 1/2⟨111] screw dislocations in BCC crystals takes place on the equivalent {110) planes.

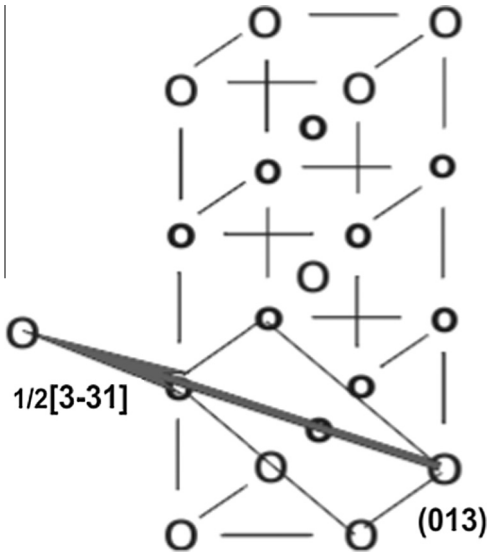

Fig. 1. Tetragonal elementary cell of $C11_b$ lattice. Large circles are metallic atoms, small circles silicon atoms. The 1/2[3$\bar{3}$1] Burgers vector and the (013) slip plane are also depicted.

As the stacking fault energy on {110) in $MoSi_2$ is significantly lower than the energies of stacking faults on {013), the dissociation widths are much larger on {110) than on {013).

The most important point is that for the loading axis along the [001] tetragonal direction, there is no shear stress acting on the {110) planes that can drive the dislocation. Hence, the transition to a {013) plane will require a large contribution of thermal activation and thus at low temperatures, such as room temperature, the deformation cannot take place and brittle fracture may ensue. This explanation is consistent with the earlier suggestion in [6].

Similarly, as in the case of 1/2⟨111] screw dislocation in the BCC structure, the 1/2 [3$\bar{3}$1] screw dislocation may dissociate in a non-planar manner on three (103), (0$\bar{1}$3) and (110) planes with similar Burgers vectors on {013), together with the 1/4⟨331] Burgers vector on (110). Due to high values of the stacking fault

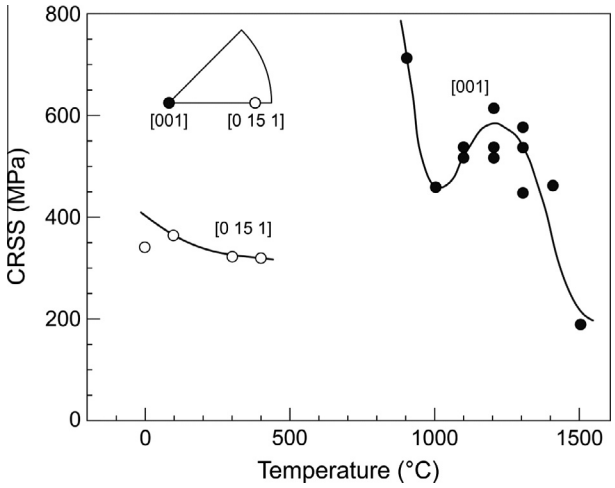

Fig. 2. Temperature dependence of the CRSS for the 1/2⟨331] slip on the {013) planes. According to [3].

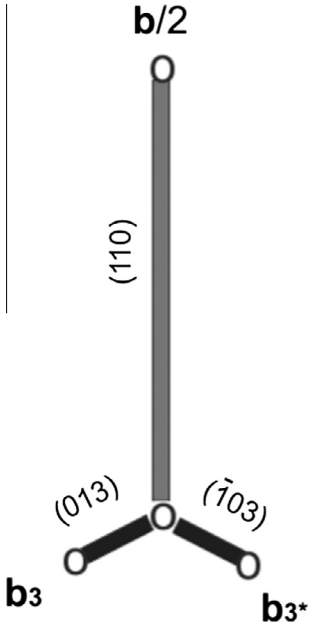

Fig. 3. Non-planar threefold splitting of 1/2[3$\bar{3}$1] dislocations on {013) and (110) planes. Circles denote the location of partial dislocations. **b** is the total Burgers vector, $\mathbf{b_3}$ and $\mathbf{b_{3*}}$ are equivalent Burgers vectors of partial dislocations on respective {013) planes.