Mo5Si3 SINGLE CRYSTALS: PHYSICAL PROPERTIES AND MECHANICAL BEHAVIOR

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Mo5Si3 Single Crystals: Physical Properties and Mechanical Behavior

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ABSTRACT

The materials processing, physical properties and mechanical behavior of an ultra-high temperature structural silicide, Mo5Si3, have been studied. High purity single crystals of Mo5Si3 have been synthesized by both optical floating zone and Czochralski methods. The thermal and elastic properties of the Mo5Si3 single crystals were experimentally measured. Results show that Mo5Si3 has significant thermal expansion anisotropy along the a and c directions with $\alpha_c/\alpha_a = 2.2$. Single crystal elastic moduli of Mo5Si3 indicate that it has less elastic anisotropy and lower shear moduli than transition metal disilicides. Tensile stresses of up to 1.8 GPa can develop at grain boundaries after cooling from the melting point due to the thermal expansion mismatch in Mo5Si3, causing grain boundary cracking during processing of polycrystals. Room temperature Vickers indentation tests on (100) and (001) planes have been performed with different indenter diagonal orientations. The orientation dependence of hardness and fracture toughness of Mo5Si3 single crystals have been obtained. The corresponding deformation and fracture modes have been revealed by microscopy studies. A comparison of Mo5Si3 with other high temperature structural silicides, e.g., C11b and C40 transition metal disilicides, is discussed.

1 Introduction

Many intermetallics and silicides offer the desired properties for high temperature structural applications, e.g., a high melting point, high strength, good oxidation resistance, and excellent creep behavior at elevated temperatures. Some candidates have been studied extensively, e.g., nickel aluminides, titanium aluminides, and transition metal disilicides. Among these phases, refractory metal silicides appear to be more attractive because of their \textit{ultra-high} melting temperatures [1]. Among the refractory metal silicides, the silicides in the Mo-Si system show promising potentials because Mo has a lower density compared to other refractory metals and Mo does not embrittle with oxygen and nitrogen volatilization. In the Mo-Si system, there are three compounds, i.e., C11b-structured MoSi2, D8m-
structured MoSi3, and A15-structured Mo3Si [2]. MoSi2 along with some transition metal disilicides has been studied extensively [1, 3–8]. Mo5Si3 and Mo3Si are receiving more attention recently in studies of their physical properties and mechanical behavior [9, 10, 11].

Mo5Si3 belongs to the space group I4/mcm (140). As a body-centered tetragonal lattice (tI32), it has 20-Mo atoms and 12-Si atoms in the unit cell. Mo5Si3 has the following structural characteristics [11]: (1) its a-lattice parameter is larger than its c-lattice parameter (a/c~2), which is different from those of typical tetragonal high temperature structural silicides, e.g., MoSi2; (2) it has no close-packed planes, which is also different from those of the typical tetragonal high temperature structural silicides, e.g., MoSi2; and (3) the -Si-Mo-Si- chains in Mo5Si3 are along [100] and [010] directions (these chains may also be along other directions, e.g., <331>) and the -Mo-Mo- and -Si-Si- chains are along [001] direction. On the other hand, the -Si-Mo-Si- chains in MoSi2 are along [001] direction and the -Mo-Mo- and -Si-Si- chains are along [100] and [010] directions. It is generally true that the interatomic bonding strength of the -Si-Mo-Si- chains is stronger than those of the -Mo-Mo- and -Si-Si- chains. Mo5Si3 has a very high melting point of 2180°C [2], which is substantially higher than that of MoSi2 (2020°C) and a reasonable density of 8.19 g/cm3, which is higher than that of MoSi2 (6.3 g/cm3). Therefore, it is considered as a promising ultra-high temperature structural material. In addition, Mo5Si3 has a relatively large range of nonstoichiometry (2-3 at.%), compared to MoSi2 which is basically a line compound, according to the Mo-Si phase diagram [2].

Initial studies for the fundamental physical properties and mechanical behavior of Mo5Si3 single crystals have been performed. In this proceedings, we report based on the previously published results [11]: (a) the synthesis of high-quality single crystals (b) the measurement of physical properties, (c) the calculation of residual thermal stresses, and (d) the mechanical behavior of Mo5Si3 single crystals.

2 Experimental Procedures and Calculation Methods

2.1 Synthesis of the Mo5Si3 Single Crystals

Elemental Mo and Si with nominal purities of 99.97 at.% and 99.95 at.% were chemically cleaned before alloying. Mo5Si3 alloys were made in the form of buttons and rods by arc-melting. Single crystals of Mo5Si3 were grown by the optical floating zone
technique using arc-melted rods and by the Czochralski method using a tri-arc crystal growth furnace and arc-melted buttons [11].

Chemical analysis was conducted for both the as-melted polycrystals and the as-grown single crystals of \( \text{Mo}_5\text{Si}_3 \). In this analysis, the Mo and Si contents were analyzed by direct current plasma emission spectroscopy. The oxygen and nitrogen contents were characterized by inert gas fusion experiments.

### 2.2 Measurement of the Physical Properties of \( \text{Mo}_5\text{Si}_3 \)

Using these \( \text{Mo}_5\text{Si}_3 \) single crystals, the thermal and elastic properties of \( \text{Mo}_5\text{Si}_3 \) were measured [11]. In the thermal property investigation, the thermal expansion of single crystal \( \text{Mo}_5\text{Si}_3 \) was examined using a Perkin-Elmer DMA-7 thermal mechanical analyzer (TMA) operated in TMA mode in the regime 298-773K. The coefficients of thermal expansion (CTE) along the \( a \) and \( c \) axes were measured on a rectangular parallelepiped specimen (5 mm [100] x 5 mm [010] x 4 mm [001]), which was cut using a diamond wafer blade from the as-grown single crystals after orienting it using the Laue back reflection technique and polished using SiC papers and lapping films. The CTE along the \( a \) axis was obtained from the measurement along the larger dimension (5 mm) and the CTE along the \( c \) axis was obtained from the measurement along the shorter dimension (4 mm).

Resonant ultrasound spectroscopy technique was employed to measure the room temperature single crystal elastic moduli of \( \text{Mo}_5\text{Si}_3 \). The single crystal \( \text{Mo}_5\text{Si}_3 \) specimen was cut and polished, as described above, into a rectangular parallelepiped geometry with dimensions \( x_1=3.217\pm0.002 \) mm, \( x_2=2.950\pm0.001 \) mm, and \( x_3=3.702\pm0.003 \) mm. The Laue back reflection x-ray technique was used to orient \( x_1 \) parallel to [100], \( x_2 \) parallel to [010] and \( x_3 \) parallel to [001]. The mass density of the specimen was determined from its dimensions and mass. The room temperature single crystal elastic moduli were determined using 70 resonant frequencies from 0.45-1.82 MHz.

### 2.3 Calculation of the Residual Thermal Stresses in \( \text{Mo}_5\text{Si}_3 \)

Using the coefficients of thermal expansion and elastic moduli of single crystal \( \text{Mo}_5\text{Si}_3 \), the residual thermal stresses developed in the solidification process are calculated for two cases. One is for a dilute concentration of particles of \( \text{Mo}_5\text{Si}_3 \) in a \( \text{Mo}_5\text{Si}_3 \) matrix using the stress associated with the elastic field related to spherical inclusions in anisotropic
solids [12, 13]. The other is for two grains of Mo$_5$Si$_3$, assuming that the interfaces can be modelled as the boundaries between two semi-infinite anisotropic solids [14].

2.4 Characterization of the Mechanical Behavior of Mo$_5$Si$_3$

Room temperature Vickers indentation tests were performed on the (100) and (001) planes of Mo$_5$Si$_3$ single crystals with different orientations of the indenter diagonal using a Micromet 4 microhardness tester. The applied load was 1 kg for 10 seconds. For each orientation of the indenter diagonal on each plane, five indents were made and the average values of the indentation impression and crack length measurements were obtained from the five indents. Using these averaged values, the Vickers hardness of Mo$_5$Si$_3$ single crystals along an orientation on a specific plane was calculated using [15]:

$$H = 1.8544 \frac{P}{d^2}$$

(3)

where $P$ is the load along the orientation on the plane the $d$ is the impression diagonal average. The corresponding indentation fracture toughness of Mo$_5$Si$_3$ was roughly estimated from [15]:

$$K = 0.016 \left( \frac{E}{H} \right)^{1/2} \frac{P}{c^{3/2}}$$

(4)

where $c$ is the radial crack length average. $E$ and $H$ are the Young’s modulus and hardness for the corresponding orientation. The impressions and cracks of the indents were further characterized using a JEOL 6300 scanning electron microscope with a field emission gun.

3 Results and Discussion

3.1 Single Crystal Fabrication

The examination using Laue back x-ray reflection patterns for the as-grown Mo$_5$Si$_3$ crystals confirmed that they are indeed single crystals [11]. Chemical analysis results for Mo, Si, O, and N are tabulated in Table 1. Table 1 indicates that the polycrystalline Mo$_5$Si$_3$ experienced some silicon loss during arc-melting, and single crystal Mo$_5$Si$_3$ had further silicon loss during crystal growth because of the silicon evaporation in these processes. However, these losses are minimal, being less than 0.5 at.%, so that the compositions of the alloys are still in the single phase region according to the Mo-Si phase diagram [2].
Using the data shown in Table 1, excess silicon can be added prior to the alloying process in order to precisely control the stoichiometry of Mo$_5$Si$_3$. It can also be found from Table 1 that the O and N impurities are very low in both polycrystalline and single crystal Mo$_5$Si$_3$ alloys, indicating that the techniques can be successfully employed to synthesize high purity Mo$_5$Si$_3$ single crystals. Using these crystals, the physical properties and mechanical behavior of Mo$_5$Si$_3$ have been investigated.

### 3.2 Physical Properties

Thermal expansions as a function of temperature along the $a=[100]$ and $c=[001]$ axes for Mo$_5$Si$_3$ single crystals were obtained [11]. The thermal expansion coefficients are essentially temperature independent over the measured temperature range. Linear curve fits of the experimental results yield the CTEs of $\alpha_a=5.2\times10^{-6}/^\circ$C and $\alpha_c=11.5\times10^{-6}/^\circ$C for Mo$_5$Si$_3$ single crystals. The coefficient of volume (bulk) expansion is $\beta=2\alpha_a+\alpha_c=21.9\times10^{-6}/^\circ$C. The most striking feature of the CTEs of Mo$_5$Si$_3$ single crystals is their strong thermal expansion anisotropy, i.e., $\alpha_c/\alpha_a=2.2$, which is substantially different from those of high temperature structural disilicides. The data in Table 2 list the thermal expansion values for Mo$_5$Si$_3$ and MoSi$_2$. It is found from Table 2 that MoSi$_2$ is almost thermally isotropic, because its value of $\alpha_c/\alpha_a$ is close to 1. Strong thermal expansion anisotropy ($\alpha_c/\alpha_a=2.2$) of Mo$_5$Si$_3$ suggests that the crystal anharmonicity is higher along the c direction in Mo$_5$Si$_3$.

The room temperature RUS spectrum of Mo$_5$Si$_3$ single crystals shows high signal-to-noise ratio and high-Q resonant peaks [11], demonstrating the high quality of the specimen and the RUS measurement. A total of 70 RUS peaks in the regime $0.45 - 1.82$ MHz were fitted and a r.m.s. error of 0.33% was obtained, indicating an excellent agreement between the experimentally measured and calculated RUS peaks. Therefore, the room temperature elastic parameters obtained from this study should be reliable.

Table 3 lists the single crystal elastic stiffness and compliance constants obtained from this study. Using these single crystal elastic parameters and formalism developed elsewhere [16, 17], the orientation dependence of the Young’s modulus of Mo$_5$Si$_3$ is plotted in Fig. 1. It was also found using these single crystal elastic parameters that: (a) the maximum Young’s modulus of Mo$_5$Si$_3$ is along the [110] direction, $E_{\text{max}}=E_{[110]}=364$ GPa, (b) the minimum Young’s modulus of Mo$_5$Si$_3$ is along the [409] direction, $E_{\text{min}}=E_{[409]}=294$ GPa, and (c) $E_{\text{max}}/E_{\text{min}}=1.24$. Therefore, Mo$_5$Si$_3$ should be the stiffest
along [110] and the most compliant along [409] in response to tension or compression loading within the elastic regime. Similarly, the orientation dependence of the shear modulus of Mo$_5$Si$_3$ is obtained and shown in Fig. 2. It can be seen from Fig. 2 that the lowest shear modulus is 110 GPa on the (001) plane along any direction, on the (100) plane along [001], and on the (110) plane along [001]. On the other hand, the shortest Burgers vector exists on the (100) plane along [001] and on the (110) plane along [001] in Mo$_5$Si$_3$, i.e., $b=[001]$. Therefore, it is reasonable to predict that the possible dislocation slip systems in Mo$_5$Si$_3$ are (100)/[001] and/or (110)/[001].

Single crystal elastic parameters can also provide valuable insight into the characteristics of interatomic bonding through certain criteria, e.g., Cauchy's relationships, elastic isotropic factors, Poisson's ratios, $c_{33}/c_{11}$ ratio, etc. The Cauchy's relationships between the elastic stiffness constants for tetragonal crystals with central forces are [18]

$$c_{13} = c_{44} \quad \text{and} \quad c_{12} = c_{66}$$

The data in Table 3 indicate that the Cauchy's relationships do not hold true for Mo$_5$Si$_3$ and this fact implies that the interatomic forces in Mo$_5$Si$_3$ are non-central. However, there are relatively less difference between $c_{13}$ and $c_{44}$ and between $c_{12}$ and $c_{66}$ for Mo$_5$Si$_3$ comparing with those of C11$_b$ and C40 transition metal disilicides [17], where the Cauchy's relationships do not hold true by more than a factor of 3 in some cases.

The elastic anisotropy factors of Mo$_5$Si$_3$ are tabulated in Table 4, along with those of MoSi$_2$. Table 4 suggests that the elastic anisotropy factors of Mo$_5$Si$_3$ are closer to unity than those of MoSi$_2$, although these factors still indicate that Mo$_5$Si$_3$ is anisotropic in elasticity.

The Poisson's ratios of Mo$_5$Si$_3$ are tabulated in Table 5, along with those of the MoSi$_2$. The data in Table 5 clearly demonstrate that the Poisson's ratios of Mo$_5$Si$_3$ single crystals are substantially larger than those of MoSi$_2$.

The $c_{33}$ and $c_{11}$ relationship of Mo$_5$Si$_3$ is different from that of C11$_b$ transition metal disilicides, e.g., MoSi$_2$ and WSi$_2$. For Mo$_5$Si$_3$, $c_{11}>c_{33}$ with $c_{33}/c_{11}=0.87$. However, for MoSi$_2$ and WSi$_2$, $c_{33}>c_{11}$ with $c_{33}/c_{11}=1.26$ [17]. This is related to the bonding strength along the [100] and [001] axes in the two intermetallic phases. As described above, the strongly bonded -Si-Mo-Si- chains are along [100] and [010] directions and the weakly bonded -Mo-Mo- and -Si-Si- chains are along [001] in Mo$_5$Si$_3$, therefore, $c_{11}$ should be larger than $c_{33}$ in this compound. On the other hand, the strongly
bonded -Si-Mo-Si- chains are along [001] and the weakly bonded -Mo-Mo- and -Si-Si-chains are along [100] and [010] directions in MoSi2 and WSi2, therefore, c33 should be larger than c11 in these phases. Furthermore, Table 3 shows that c11+c12>c33 for Mo5Si3. c11+c12>c33 suggests that the elastic tensile modulus is larger on the (001) plane than along the [001] direction. This indicates that the bonding in the (001) plane is stronger than the bonding along the [001] direction for Mo5Si3. In fact, these results of bonding analysis in Mo5Si3 are consistent with the thermal expansion anisotropy (αc/αa=2.2) of Mo5Si3. First-principles total energy and electronic structure calculations have confirmed these results, yielding more detailed information about interatomic bonding for Mo5Si3 [19].

The isotropic elastic moduli of Mo5Si3 can be derived by the Voigt, Reuss, or Hill approximation and compared with those of the constituent elements and the average values derived from the rule of mixtures. These values are given in Table 6. It can be seen that the isotropic elastic moduli and the Poisson's ratio of polycrystalline Mo5Si3 are close to those of Mo, especially the shear and Young's moduli. The rule of mixtures does not hold true for Mo5Si3. The Poisson's ratio of polycrystalline Mo5Si3 is 0.278 as shown in Table 6, which is substantially larger than ν ~ 0.15 of the C11b transition metal disilicides and ν ~ 0.19 of the C40 transition metal disilicides [17].

The specific Young's modulus (the ratio of the Young's modulus to the density of a material) is an important engineering design parameter for materials in aerospace applications. Figure 3 demonstrates the specific Young's moduli of high temperature structural silicides. It can be seen from Fig. 3 that the specific Young's modulus of Mo5Si3 is in general smaller than those of transition metal disilicides, but higher than those of nickel aluminides (25-32 GPa/(g/cm³)) and comparable with those of titanium aluminides (30-50 GPa/(g/cm³)).

3.3 Residual Thermal Stress

Figure 4 shows the residual thermal stress due to a spherical grain of Mo5Si3 in a matrix of Mo5Si3 with a misorientation such that the thermal expansion mismatch is maximized. It can be seen that the tensile stress in the Mo5Si3 matrix can reach a maximum of about 1.8 GPa during the cooling from the melting point.

In the calculation of the residual thermal stress next to a planar interface of two Mo5Si3 grains, the stresses is calculated as a function of misorientation of the two grains
characterized by $\theta_1$ and $\theta_2$, as shown in Fig 5. Figure 6 demonstrates that a maximum of up to 1 GPa thermal stress can develop near a planar interface of two grains with certain misorientation in Mo$_5$Si$_3$.

Although it is not practical to calculate the residual thermal stresses for all possible cases, the two calculations for the two typical cases clearly demonstrate that substantially high residual thermal stresses, up to 1.8 GPa, can develop in Mo$_5$Si$_3$ due to thermal expansion mismatch between different grains. These large stresses, which are obviously higher than the compression and tension strength, can fracture weakly bonded grain boundaries in the solidification process, unless other mechanisms to relieve these stresses are operative, such as dislocation plasticity, twinning formation, stress induced phase transformation, etc. Indeed, significant grain boundary cracking was observed in the arc-melted buttons and rods used in this study. Therefore, the Mo$_5$Si$_3$-based materials can only be properly studied and/or applied using: (a) single crystals, (b) polycrystals with very smaller grain sizes, or (c) Mo$_5$Si$_3$ properly alloyed by some elements, e.g., boron, to avoid the grain boundary cracking problem [21, 22].

3.4 Mechanical Behavior

The orientation dependence of the room temperature Vickers hardness, calculated from Eq. (3), on the (100) and (001) planes of Mo$_5$Si$_3$ single crystals is shown in Fig 7 (a). The hardness on these planes of Mo$_5$Si$_3$ is not significantly orientation dependent and the hardness has large values around 1200 kg/mm$^2$, which are substantially higher than those of MoSi$_2$ single crystals (600-900 kg/mm$^2$, depending on the testing orientations) [23] and those of NbSi$_2$ single crystals (~700 kg/mm$^2$, depending on the testing orientations) [24]. It is interesting to note that there is a noticeable difference (~10%) between the hardness on the same (001) plane but with different indenter diagonal orientations.

Figure 7 (b) demonstrates the orientation dependence of the indentation fracture toughness, roughly estimated from Eq. (4), on the (100) and (001) planes of Mo$_5$Si$_3$ single crystals. It can be seen from Fig. 7 (b) that the room temperature indentation fracture toughness on these planes of Mo$_5$Si$_3$ is within 2-2.5 MPa$\sqrt{m}$, showing a minor orientation dependence. These values are comparable with those of MoSi$_2$ single crystals on some orientations [23]. It is also interesting to note that there is a noticeable difference (~10%)
between the fracture toughness on the same (001) plane but with different indenter diagonal orientations.

SEM micrographs of the indentation impressions and the associated cracks on the (100) and (001) planes with two indenter diagonal orientations are shown in Fig. 8. Dislocation slip traces are not observed near the indent impressions, suggesting that dislocation slip may not be operative for these mechanical loading at ambient temperature in Mo5Si3. Figure 8 also demonstrates that the cracks are generated at the four-corners of the indent impression and no secondary cracks are observed for Mo5Si3. On the other hand, cracks may be generated at only two corners of some indent impressions and substantial secondary cracks are observed for MoSi2 [23]. Therefore, the fracture behavior of Mo5Si3 may be less anisotropic than that of MoSi2. The significant feature is that the indentation shapes for the two different indenter diagonal orientations on the (001) plane are completely different, as shown in Fig. 8 (c) and (d). This may be responsible for the noticeable differences (~10%) in the hardness and fracture toughness for these indentations as mentioned above. It is important to understand the reason(s) why such a significant difference exists in the plastic response to the same loading by considering the elastic properties and examining the plastic deformation mechanisms in Mo5Si3.

4 Conclusions

The physical properties and mechanical behavior of Mo5Si3 single crystals have been studied. Four primary conclusions have been reached:

(1) Mo5Si3 single crystals with minimal oxygen and nitrogen impurities (~10 wppm) have been synthesized by both the optical floating zone and the Czochralski methods. Silicon loss in alloy processing and single crystal growth is less than 0.5 at. %.

(2) Thermal and elastic properties of Mo5Si3 single crystals have been experimentally measured. Mo5Si3 has the CTEs of \( \alpha_a = 5.2 \times 10^{-6} / ^\circ C \) and \( \alpha_c = 11.5 \times 10^{-6} / ^\circ C \), showing a strong thermal expansion anisotropy (\( \alpha_c/\alpha_a = 2.2 \)). Mo5Si3 has room temperature single crystal elastic constants of \( c_{11} = 446 \), \( c_{33} = 390 \), \( c_{13} = 140 \), \( c_{12} = 174 \), \( c_{44} = 110 \), and \( c_{66} = 140 \) GPa, respectively. Analysis of the elastic parameters reveals that the bonding in the (001) plane is stronger than the bonding along the [001] direction and the crystal anharmonicity is higher along the [001] direction for Mo5Si3.
(3) Significantly large residual thermal stresses (up to 1.8 GPa) can develop in Mo₅Si₃ in the solidification process due to thermal mismatch between different grains, causing grain boundary cracking.

(4) Room temperature Vickers indentation tests on the (100) and (001) planes reveal that Mo₅Si₃ have a hardness of around 1200 kg/mm² and a fracture toughness above 2 MPa√m. Plastic responses (the shape of indent impression) to the (001) indentations with two different indenter diagonal orientations are significantly different, resulting in a noticeable difference in the corresponding hardness and fracture toughness.

Acknowledgments

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References


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22  C. T. Liu, J. Schneible, and M. H. Yoo, *private communications*.


Figure Captions

Figure 1  The orientation dependence of the Young's modulus of Mo$_5$Si$_3$ single crystals: (a) the 3-dimensional plot, (b) the Young's moduli along the directions perpendicular to [001], and (c) the Young's moduli along the directions perpendicular [100] (from Ref. [11]).

Figure 2  The orientation dependence of the shear moduli of Mo$_5$Si$_3$ single crystals on the (001) plane from [110] to [010], the (100) plane from [001] to [010], and the (110) plane from [001] to [110] (from Ref. [11]).

Figure 3  Specific Young's modulus of high temperature structural silicides.

Figure 4  Stresses for a spherical grain of Mo$_5$Si$_3$ embedded in a matrix of Mo$_5$Si$_3$ misoriented such that the thermal expansion mismatch is maximized. (a) matrix; (b) grain.

Figure 5  Initial crystallography and rotation scheme to calculate residual thermal stresses in a planar interfaces as a function of misorientation.

Figure 6  Thermal stresses (in MPa) for a planar interface shown in Fig. 4 as a function of the misorientation. (a) $\sigma_{11}$; (b) $\sigma_{22}$.

Figure 7  The orientation dependence of (a) the room temperature Vicker's hardness and (b) the indentation fracture toughness on the (100) and (001) planes of Mo$_5$Si$_3$ single crystals. (100)[011] means the indentation is on the (100) plane and one indenter edge is parallel to [011] (from Ref. [11]).

Figure 8  SEM micrographs of the indentation impressions and the associated cracks on Mo$_5$Si$_3$ single crystals: (a) on the (100) plane and one indenter edge is parallel to [011], (b) on the (100) plane and one indenter edge is parallel to [010], (c) on the (001) plane and one indenter edge is parallel to [110], and (d) on the (001) plane and one indenter edge is parallel to [100] (from Ref. [11]).
## Tables

**Table 1** Chemical analysis results of the Mo₅Si₃ alloys (from Ref. [11]).

<table>
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<tr>
<th></th>
<th>Mo (at.%)</th>
<th>Si (at.%</th>
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<th>N (wppm)</th>
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**Table 2** The thermal expansion data of Mo₅Si₃ and MoSi₂.

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<th>$\alpha_c$ ($10^{-6}/°C$)</th>
<th>$\beta$ ($10^{-6}/°C$)</th>
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**Table 3** Room temperature elastic stiffness and compliance constants of Mo₅Si₃ single crystals (from Ref. [11]).

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<th>(i,j)</th>
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<th>12</th>
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<td>$c_{ij}$ (GPa)</td>
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**Table 4** Elastic anisotropy factors of Mo₅Si₃ and MoSi₂.

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<th>Anisotropy Factors</th>
<th>Mo₅Si₃</th>
<th>MoSi₂</th>
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<tbody>
<tr>
<td>$c_{33}/c_{11}$</td>
<td>0.874</td>
<td>1.255</td>
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<tr>
<td>$c_{13}/c_{12}$</td>
<td>0.804</td>
<td>0.796</td>
</tr>
<tr>
<td>$2c_{44}/(c_{11}-c_{12})$</td>
<td>0.809</td>
<td>1.401</td>
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<td>$2c_{66}/(c_{11}-c_{12})$</td>
<td>1.029</td>
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Table 5 The Poisson's ratios of Mo₅Si₃ and MoSi₂.

<table>
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<td>v₃₁ = -s₁₃/s₃₃</td>
<td>0.2255</td>
<td>0.1780</td>
</tr>
<tr>
<td>v₁₂ = -s₁₂/s₁₁</td>
<td>0.3107</td>
<td>0.2570</td>
</tr>
<tr>
<td>v₁₃ = -s₁₃/s₁₁</td>
<td>0.2464</td>
<td>0.1360</td>
</tr>
</tbody>
</table>

Table 6 The isotropic elastic moduli and Poisson's ratio of Mo₅Si₃. K is the bulk modulus, G the shear modulus, E the Young's modulus, and v the Poisson's ratio (from Ref. [11]).

<table>
<thead>
<tr>
<th>Materials</th>
<th>K (GPa)</th>
<th>G (GPa)</th>
<th>E (GPa)</th>
<th>v</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mo (a)</td>
<td>259.7</td>
<td>125.0</td>
<td>323.2</td>
<td>0.293</td>
</tr>
<tr>
<td>Si (a)</td>
<td>97.9</td>
<td>68.1</td>
<td>162.9</td>
<td>0.225</td>
</tr>
<tr>
<td>Mo₅Si₃: Averaged Values</td>
<td>199</td>
<td>104</td>
<td>263</td>
<td>0.268</td>
</tr>
<tr>
<td>Mo₅Si₃: Hill Approximation</td>
<td>242</td>
<td>126</td>
<td>323</td>
<td>0.278</td>
</tr>
</tbody>
</table>

(a) compiled from the data in Ref. [20].
Figure
Figure

Shear Modulus (GPa) vs. Orientation, Theta (deg.)

- (001) from [100] to [010]
- (100) from [001] to [010]
- (110) from [001] to [110]
Specific Young's Modulus (GPa/(g/cm$^3$))

- $\text{Me}_5\text{Si}_3$: 8
- ReSi$_2$: 7
- WSi$_2$: 6
- MoSi$_2$: 5
- CrSi$_2$: 4
- TaSi$_2$: 3
- NbSi$_2$: 2
- VSi$_2$: 1
\[
\sigma^{\text{grain}} = \begin{pmatrix}
1840 & 0 & 0 \\
0 & -1840 & 0 \\
0 & 0 & 0
\end{pmatrix} \text{ [MPa]}
\]

Figure
Figure

(a)

(b)
Figure
Fracture Toughness [MPa.m$^{1/2}$]

Orientation

(100)[011] (100)[010] (001)[110] (001)[100]