Elastic properties and stacking fault energies of Cr$_2$Ta

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Dedicated to Dr. Gerhard Sauthoff on the occasion of his 60th birthday

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Abstract

The elastic moduli, stacking fault and twin boundary energies of C15 Cr$_2$Ta are calculated by first-principles local-density-functional approach. Similarly to the case of Cr$_2$Nb, Cr$_2$Ta is characterized by a low twin boundary energy (33 mJ/m$^2$). On the other hand, the intrinsic and extrinsic stacking fault energies are found to be 88 and 83 mJ/m$^2$, respectively. Using the results of elastic constants and stacking fault energies, we predict the equilibrium separation between Shockley partials. The results of Cr$_2$Ta are compared with those of Cr$_2$Nb.

Keywords: A. Laves phase; B. Elastic properties

1. Introduction

Cr$_2$Ta is one of Laves phase compounds, which have attractive properties such as high-melting temperature, low density, and high oxidation resistance for structural applications. Mainly due to low temperature brittleness, this potential has not been well exploited.

To understand the brittle fracture behavior and deformation mechanism, we need to know some basic properties such as elastic constants and stacking fault energies (SFEs), $\gamma_{SF}$, since these are important factors that control deformation processes such as dislocation dissociation, cross-slip, and twin formation.

In this paper, we present the theoretical predictions of elastic moduli, and stacking fault and twin boundary energies of Cr$_2$Ta. Using the results of elastic constants and stacking fault energies, we also predict the equilibrium separation between Shockley partials. These results of Cr$_2$Ta are compared with those of Cr$_2$Nb, which was studied in our previous papers [1,2].

2. Elastic properties

Total-energy calculations for C15 Cr$_2$Ta were performed using the full-potential linearized augmented plane-wave (FLAPW) method within the local-density approximation. The FLAPW method solves the local-density-functional equations without any shape approximation to the potential or charge density. The atomic positions were relaxed by calculating Hellmann–Feynman forces acting on the atoms.

The theoretical lattice constant 6.809 Å of C15 Cr$_2$Ta was obtained, which is in good agreement with the experimental lattice constant 6.985 Å [3]. Next, we calculated the elastic constants. Similarly as in Ref. [1], three independent elastic constants ($C_{11}$, $C_{12}$, and $C_{44}$) are determined from three relations of the energy density $U$: (i) $U = (C_{11} - C_{12})e^2$ for $e_1 = -e_2 = e$, (ii) $U = (C_{11} + C_{12})e^2$ for $e_1 = e_2 = e$, and (iii) $U = 2C_{44}e^2$ for $e_6 = e$, where $e_i$’s are the strain components, by fitting the calculated values to third-order polynomials. The results are shown in Table 1: $C_{11}$ and $C_{44}$ of Cr$_2$Ta are larger than those of Cr$_2$Nb, while $C_{12}$ is rather close to that of Cr$_2$Nb. The difference in the elastic constants at theoretical and experimental volumes is due to the lattice anharmonicity.

In order to compare the elastic moduli of polycrystals, we calculate bulk, shear and Young’s moduli of C15 Cr$_2$Ta. To our knowledge, there has been no published experimental measurements on the elastic moduli. Table 2 shows the Hill’s averages of elastic moduli of Cr$_2$Ta, along with those of Cr$_2$Nb. The Hill’s average is the arithmetic mean of the Voigt average and Reuss average [1]. The elastic moduli of Cr$_2$Ta are larger than those of Cr$_2$Nb, which is consistent with the fact that Cr$_2$Ta (2020°C [4]) has a higher melting point than Cr$_2$Nb (1730°C [5]).

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Table 1
Three calculated elastic constants (in units of GPA) at both theoretical and experimental volumes for C15 Cr2Ta

<table>
<thead>
<tr>
<th></th>
<th>C11</th>
<th>C12</th>
<th>C44</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr2Ta</td>
<td>360</td>
<td>220</td>
<td>94</td>
</tr>
<tr>
<td></td>
<td>281</td>
<td>173</td>
<td>73</td>
</tr>
<tr>
<td>Cr2Nb (Ref. [1])</td>
<td>250</td>
<td>170</td>
<td>58</td>
</tr>
</tbody>
</table>

Table 2
Elastic moduli derived from three elastic constants at both theoretical and experimental volumes. A, B, E, G, and υ represent elastic anisotropy ratio, bulk modulus, Young’s modulus, shear modulus and Poisson’s ratio, respectively

<table>
<thead>
<tr>
<th></th>
<th>A (GPa)</th>
<th>B (GPa)</th>
<th>E (GPa)</th>
<th>G (GPa)</th>
<th>υ</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr2Ta</td>
<td>1.35</td>
<td>267</td>
<td>226</td>
<td>83</td>
<td>0.359</td>
</tr>
<tr>
<td></td>
<td>1.34</td>
<td>209</td>
<td>175</td>
<td>64</td>
<td>0.360</td>
</tr>
<tr>
<td>Cr2Nb (Ref. [1])</td>
<td>1.45</td>
<td>197</td>
<td>138</td>
<td>50</td>
<td>0.383</td>
</tr>
</tbody>
</table>

3. Stacking geometry of Laves structures

The Laves structures (C15, C14, and C36) have the formula SN where S and L represent smaller and larger atoms, respectively. They can be considered as having three different kinds of stacking sequences: C15 is XYZ stacking along the (111) direction, and C14 is X’Z stacking along the (0001) direction, and C36 is XYZ/′Y′ stacking along the (0001) direction, in the topologically close-packed structure. Each X, Y, or Z unit consists of the quadruple atomic layers. For atomic layers, there are two types of atomic stacking sequences, aαaβ (ββα and γγγγ) and acbβ (ββy and yγα). Here, the Greek letters (α, β, γ) denote the larger L atoms, while lowercase Latin letters (a, b, c) and capital letters (A, B, C) denote the type-1 and type-2 smaller S atoms, respectively. In terms of stacking sequences, the C15, C14, and C36 are defined as follows:

\[C15 : \ldots Aa\bar{a}b\bar{a}yC\bar{y}a\ldots\]  
\[C14 : \ldots Aab\bar{y}Cy\bar{a}\ldots\]  
\[C36 : \ldots AacbB\bar{b}yCy\bar{a}\beta\alpha\ldots\]

The primed units (X’, Y’, Z’) are introduced by synchroshear [6] in order to make sure that a topologically close-packed (TCP) structure is preserved in C14 and C36. For example, c and β of X unit in C15 are synchrosheared to become b and γ of X’ unit, respectively.

The stacking sequences for intrinsic stacking fault (ISF) and extrinsic stacking fault (ESF) and twin boundary are given in Table 3 in terms of X, Y, and Z units. For ISF, one unit, namely Y, is missing from the C15 XYZ sequence and X becomes X’ by synchroshear. For ESF, a unit Y’ is added into the C15 sequence, and consequently two primed units (Z’ and Y’) are introduced by two successive synchroshears in the acβ types. Twinned structure is a mirror reflection about the X’ unit (see Table 3).

4. Stacking fault and twin boundary energies

The supercell geometry is used to obtain the energies of ISF, ESF and twin boundary. We consider a supercell containing XYZ’Z for ISF and XYZXYZ’Y’ for ESF, while a supercell containing XYZXYZ’Y is considered for twin boundary.

In the supercell calculation, we use the experimental lattice constant (6.985 Å) of C15 Cr2Ta and spacings along a, axis corresponding to the ideal hcp c/a ratio, which gives ~4.03 Å for the thickness of each X, Y, or Z unit. Similarly to the Cr2Nb case, the separations between ISF and ESF planes in the supercells are about 20 and 28 Å, respectively, and the separation between twin boundaries is about 12 Å. The internal coordinates of each structure are fully relaxed from the ideal positions (defined by the atomic positions of the C15 lattice) by calculating Hellmann–Feynman forces acting on the atoms. The relaxation energies of ISF, ESF, and twin boundary are 36, 33, and 15 mJ/m², respectively.

The results for the stacking fault and twin boundary energies are given in Table 4. It is found that the fault energies are γSF = 88 and γESF = 83 mJ/m² for ISF and ESF, respectively, and the twin boundary energy is γT = 33 mJ/m². These results are smaller than those of Cr2Nb (see Table 4).

Table 3
Stacking sequences of the C15 structure (no stacking fault), intrinsic stacking fault, extrinsic stacking fault, and twin structure

<table>
<thead>
<tr>
<th>Sequence of faults</th>
<th>C15</th>
<th>Intrinsic stacking fault</th>
<th>Extrinsic stacking fault</th>
<th>Twin (C15+C15T)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>...XYZXYZXYZ...</td>
<td>...XYZXYZXYZ...</td>
<td>...XYZXYZXYZ...Y...</td>
<td>...XYZXYZXYZ...Y...</td>
</tr>
</tbody>
</table>

Table 4
Stacking fault and twin boundary energies for C15 Cr2Ta and Cr2Nb, using the experimental lattice constant

<table>
<thead>
<tr>
<th></th>
<th>γSF (mJ/m²)</th>
<th>γT (mJ/m²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cr2Ta</td>
<td>88 (intrinsic)</td>
<td>83 (extrinsic)</td>
</tr>
<tr>
<td>Cr2Nb (Ref. [2])</td>
<td>116 (intrinsic)</td>
<td>94 (extrinsic)</td>
</tr>
</tbody>
</table>
5. Interaction between Shockley partials

From the anisotropic elasticity theory [7,8] we calculate the equilibrium separation between Shockley partials, using the calculated elastic constants and stacking fault energies. For ISF, the Burgers vector \( \frac{1}{2} [110] \) dissociates into two Shockley partials:

\[
\frac{1}{2} [1\bar{1}0] \to \frac{1}{6} [1\bar{2}1] + \text{ISF} + \frac{1}{6} [2\bar{1}1].
\]

(4)

The equilibrium separation between the partials can be obtained through the balance of the attractive force (the surface tension due to ISF) and the repulsive force (due to elastic interaction between the partials).

The width of the equilibrium separation, \( w \), can be obtained from

\[
w = f_r/(2\pi \gamma_{\text{SF}}),
\]

(5)

where \( f_r \) is the radial (in the \( \{111\} \) plane) component of the interaction force constants, which are determined from the anisotropic elasticity theory of dislocations [7], and obtained numerically [9]. The separation is \( w_s = 32.0 \text{ Å} \) for the \( \mathbf{B} = \frac{1}{2} [110] \) screw dislocation, and \( w_e = 88.6 \text{ Å} \) for the edge dislocation. These results are shown in Table 5.

For the isotropic approximation, the equilibrium separation \( w \) is given by [8]

\[
w = \frac{G\beta^2}{8\pi \gamma_{\text{SF}}} \frac{2 - \nu}{1 - \nu} \left( 1 - \frac{2\nu \cos 2\phi}{2 - \nu} \right).
\]

(6)

where \( \phi \) is the angle between a dislocation line and the Burgers vector \( \mathbf{B} \). It is found that \( w_s = 34.2 \text{ Å} \) and \( w_e = 87.7 \text{ Å} \). As given in Table 5, the results in anisotropic and isotropic cases are very close to each other.

For the dissociation of \( \frac{1}{2} [110] \) into partials bounding ESF, it is found that \( w_s = 33.9 \text{ Å} \), and \( w_e = 93.9 \text{ Å} \) for the anisotropic case, while \( w_s = 36.3 \) and \( w_e = 92.9 \text{ Å} \) for the isotropic case.

On the other hand, we consider the separation between partials by using the theoretical lattice constant. For ISF, the separation is \( w_s = 29.6 \text{ Å} \) and \( w_e = 81.5 \text{ Å} \) for the anisotropic case, while \( w_s = 31.7 \text{ Å} \) and \( w_e = 80.6 \text{ Å} \) for the isotropic case. For ESF, the separation is \( w_s = 35.7 \text{ Å} \) and \( w_e = 98.3 \text{ Å} \) for the anisotropic case, while \( w_s = 38.2 \text{ Å} \) and \( w_e = 97.3 \text{ Å} \) for the isotropic case. It can be seen that the separations are very close for using both experimental and theoretical lattice constants.

Compared with the results of Cr2Nb (see Table 5), we found that the separations for Cr2Ta are larger than those of Cr2Nb by a factor of 1.4–1.8. This may imply that dislocations in Cr2Ta move more easily than those in Cr2Nb; giving rise to a relatively more planar slip when it occurs.

6. Summary

We performed first-principles total-energy calculations to obtain the elastic moduli, and stacking fault and twin boundary energies of C15 Cr2Ta. The elastic constants and moduli were calculated. The intrinsic and extrinsic stacking fault energies were found to be 88 and 83 mJ/m², respectively, and the twin boundary energy is 33 mJ/m². We predicted the equilibrium separations between Shockley partials using the calculated elastic constants and stacking fault energies. As far as we know, there has been no experimental data on elastic moduli and stacking fault energies of C15 Cr2Ta, with which we can compare our theoretical results.

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References