The influence of temperature on the mechanical properties of polycrystalline and single-crystalline Ni₃Al

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Abstract. Because of the excellent mechanical property at high temperature, single-crystalline Ni₃Al-based alloys, which belong to Ni-based superalloys, are widely adopted in the fields of aerospace, aviation and military. Usually, single-crystalline Ni-based alloys are bonded or welded together by polycrystalline Ni-based alloys. In this study, the Young’s modulus, shear modulus, bulk modulus, and Poisson ratio of polycrystalline Ni₃Al at the temperature ranging from 10 ℃ to 850 ℃ were calculated according to Voigt – Reuss approximation, and the relationships between the mechanical properties and the temperatures were clarified. Moreover, the influence of temperature on the universal anisotropy index and mechanical properties of single-crystalline Ni₃Al was evaluated. Results show that, except for Poisson ratio, the increase of temperature linearly decreases the mechanical properties of polycrystalline Ni₃Al, while it increases the universal anisotropy index of the single-crystalline Ni₃Al. Moreover, different with the bulk modulus, the Young’s modulus and shear modulus of single-crystalline Ni₃Al are obvious anisotropic, and their anisotropic characteristics are quite opposite. The increasing temperature decreases both maximum and minimum values of Young’s modulus, shear modulus, and bulk modulus of single-crystalline Ni₃Al.

1. Introduction
For the excellent mechanical and physical properties at high temperatures, such as extremely high strength, creep limit, fatigue limit, corrosion and oxidation resistances, nickel(Ni)-based superalloys are widely used in the fields of aerospace, aviation and military [1-3]. As surface imperfections, grain boundaries inevitably weaken the mechanical and other properties of metal at high temperatures. Accordingly, the latest generation of Ni-based superalloys are single crystals. Because of the poor forming performance of single-crystalline Ni-based superalloys and the complicated shape of parts or components, single-crystalline Ni-based alloys (i.e., parent alloy) are usually bonded or welded together by polycrystalline Ni-based alloys (i.e., intermediate layer) [4-6]. The state of the crystallographic orientation in the single-crystalline parent alloy are totally different with that in the polycrystalline intermediate layer. Although some mechanical properties of polycrystalline Ni-based alloys have been measured by experimental measurement, the influence of temperature on the mechanical properties is still not investigated systematically [7-9]. In addition, because of crystal anisotropy, there are countless crystal orientations in a single crystal, and the mechanical properties of single-crystalline Ni-based alloys in three-dimensional space are impossible to be measured by experimental method. In the previous study [10], first-principles calculations based on density function theory (DFT) were employed to calculate the mechanical properties of alloy in all crystal orientations,
and the calculation results could be verified by experimental data. However, for the limitation of DFT, the influence of temperature on the mechanical properties of single-crystalline alloys cannot be investigated via first-principles calculations. The authors’ latest study shows that the differences of the mechanical properties induced by different states of crystal orientations between the single-crystalline parent alloy and polycrystalline intermediate layer induce stress and strain concentration in the bonding or welded joints [11]. Thus far, in-depth and systematic comparative studies of single-crystalline and polycrystalline Ni-based superalloys are very scarce, especially for these at various temperatures.

Ni3Al is a kind of intermetallic compound. Ni3Al-based alloys, which have outstanding mechanical and physical performances, belong to the Ni-based superalloys. In the present study, the mechanical properties of single-crystalline and polycrystalline Ni3Al were calculated, and the influence of temperature on the mechanical properties of polycrystalline and single-crystalline Ni3Al was clarified.

2. Computational methods

Intermetallic compound Ni3Al has a face-centered cubic lattice structure and Pm-3m space group, and its lattice constant is \( a = 3.572 \) Å, as shown in Figure 1(a) [12]. Considering the lattice symmetry of cubic structure, the stiffness matrix of single-crystalline Ni3Al can be expressed as:

\[
\begin{bmatrix}
\sigma_1 \\
\sigma_2 \\
\sigma_3 \\
\tau_1 \\
\tau_2 \\
\tau_3
\end{bmatrix}
= 
\begin{bmatrix}
C_{11} & C_{12} & C_{13} & 0 & 0 & 0 \\
C_{22} & C_{23} & 0 & 0 & 0 & \varepsilon_2 \\
C_{33} & 0 & 0 & 0 & \varepsilon_3 \\
C_{44} & 0 & 0 & \gamma_1 \\
C_{55} & 0 & \gamma_2 \\
C_{66} & \gamma_3
\end{bmatrix}
\]

Where \( \sigma, \tau, \varepsilon, \gamma \) are the normal stress, shearing stress, and the corresponding normal strain and shearing strain, respectively. The inverse matrix of stiffness matrix \([C]\) is the flexibility matrix \([S]\), and there are three independent variables \((C_{11}, C_{44}, C_{12}, \text{and } S_{11}, S_{44}, S_{12})\) in them, respectively, because of the lattice symmetry of cubic structure. The values of the independent variables ranging from 10 \( ^\circ C \) to 850 \( ^\circ C \) can be obtained from a previous study [13]. For a cubic lattice, according to the Voigt–Reuss approximation [14], the upper limits of bulk modulus \((B_V)\) and shear modulus \((G_V)\) can be calculated by Equation (1) and Equation (2), respectively:

\[
B_V = \frac{1}{3}(C_{11} + 2C_{12})
\]

\[
G_V = \frac{1}{5}(C_{11} - C_{12} + 3C_{44})
\]

The lower limits of bulk modulus \((B_R)\) and shear modulus \((G_R)\) are written as Equation (3) and Equation (4), respectively:

\[
B_R = \frac{1}{3}(C_{11} + 2C_{12})
\]

\[
G_R = \frac{5(C_{11} - C_{12})C_{44} + 3(C_{11} - C_{12})}{4C_{44} + 3(C_{11} - C_{12})}
\]

The practical bulk modulus \((B)\) and shear modulus \((G)\) are estimated as the arithmetic mean, as given in Equation (5) and Equation (6), respectively:
\[ B = \frac{1}{2}(B_R + B_V) \]  
(5)

\[ G = \frac{1}{2}(G_R + G_V) \]  
(6)

Then, Young’s modulus \(E\) and Poisson ratio \(v\) can be calculated by Equation (7) and Equation (8), respectively:

\[ E = \frac{9BG}{3B + G} \]  
(7)

\[ v = \frac{3B - E}{6B} \]  
(8)

The elastic anisotropy of single-crystalline Ni$_3$Al can be described by the universal anisotropy index \(A_U\) [15], which can be expressed as

\[ A_U = 5 \frac{G_V}{G_R} + \frac{B_V}{B_R} - 6 \]  
(9)

To further understand the anisotropic mechanical properties of single-crystalline Ni$_3$Al, the Young’s modulus \(E\) and bulk modulus \(B\) in all crystal orientations can be expressed as [16]

\[ \frac{1}{E} = \left( S_{11} - S_{12} - \frac{S_{44}}{2} \right) \left( l_1^2 l_2^2 + l_2^2 l_3^2 + l_3^2 l_1^2 \right) \]  
(10)

\[ \frac{1}{B} = \left( S_{11} + 2S_{12} \right) \left( l_1^2 + l_2^2 + l_3^2 \right) \]  
(11)

Where \(l_1, l_2,\) and \(l_3\) denote the direction cosines with respect to the \(a, b,\) and \(c\) axis (i.e., directions [100], [010], and [001]) of the lattice. The shear modulus \(G\) in all crystal orientations can be expressed as Equation (12):

\[ \frac{1}{G} = \left( S_{44} + 4S_0 J \right), \quad \text{and} \quad J = \sin^2 \theta \cdot \cos^2 \phi + 0.125 \cdot \sin^4 \theta (1 - \cos 4\phi), \]  
(12)

Where \(\theta\) and \(\phi\) are Euler angles in the direction cosines, see Figure 1(b).

![Figure 1](image)

**Figure 1.** The structures of cubic Ni$_3$Al: (a) unit cell; and (b) coordinates system and Eulerian angles.
3. Results and discussion

Figure 2 shows the temperature dependences of the mechanical modulus and Poisson ratio of the polycrystal Ni₃Al at various temperature. Clearly, the Young’s modulus, shear modulus, and bulk modulus of the polycrystalline Ni₃Al decrease linearly with the increase of temperature, see Figure 2(a). By linear fitting, the relations between these moduli and the temperature (T) can be expressed as:

\[ E = 1.92832 \times 10^{11} - 5.08373 \times 10^{7} T, \quad R^2 = 99.8 \]
\[ G = 7.8808 \times 10^{10} - 2.16755 \times 10^{7} T, \quad R^2 = 99.8 \]
\[ B = 1.16147 \times 10^{11} - 2.4362 \times 10^{7} T, \quad R^2 = 98.9 \]  

Generally, Poisson ratio rises with the increasing temperature. However, different with the Young’s modulus, shear modulus and bulk modulus, there is no obvious linear relation, see Figure 2(b). For example, the Poisson ratio will decrease obviously when the temperature is higher than 750 °C.

The arrangement characteristics of atom determine the mechanical anisotropy of material, which has a significant influence on the mechanical behaviour, e.g., crack growth, anisotropic deformation and elastic instability. Figure 3 exhibits the temperature dependence of universal anisotropy index in the single-crystalline Ni₃Al. Clearly, increasing temperature linearly increases the universal anisotropy index \( A_U \) of the single-crystalline Ni₃Al, which can be expressed as Equation (16) by linear fitting:

\[ A_U = 1.61426 + 2.74628 \times 10^{-4} T, \quad R^2 = 99.9 \]  

![Figure 2](image1.png)

**Figure 2.** The temperature dependences of mechanical modulus (a) and Poisson ratio (b) of the polycrystalline Ni₃Al.

![Figure 3](image2.png)

**Figure 3.** The temperature dependence of universal anisotropy index in the single-crystalline Ni₃Al.

Orientation dependences of Young’s modulus in the single-crystalline Ni₃Al are illustrated in Figures 4(a1)–(a3), where in the maximum Young’s moduli are in the directions <111> and the minimum Young’s moduli are along the three axes (i.e., <100> directions) at various temperatures. Moreover, Figures 4(b1)–(b3) reveal that, contrary to the directional dependence of Young’s modulus, the values of all shear modulus along directions <100> are maximal, while the minimum shear moduli
are all located at directions <111>. Therefore, both the Young’s modulus and shear modulus of single-crystalline Ni$_3$Al show obvious anisotropic characteristics, and they are quite opposite. Nevertheless, there is no anisotropic phenomenon for bulk modulus, i.e., the value of bulk modulus in all orientations is same at a given temperature, and the maximum bulk modulus equals to the minimum bulk modulus, see Figures 4(c1)–(c3). Figure 5 shows the influence of temperature on the maximum and minimum modulus of Young’s modulus, shear modulus, and bulk modulus. Approximatively, both maximum and minimum values decrease linearly with the increase of temperature, and the maximum and minimum values at 10 °C, 400 °C and 850 °C are listed in Table 1.

![Figure 4](image1.png)

**Figure 4.** Crystal direction dependences of mechanical property in the single-crystalline Ni$_3$Al: (a1) Young’s modulus, 10 °C; (a2) Young’s modulus, 400 °C; (a3) Young’s modulus, 850 °C; (b1) shear modulus, 10 °C; (b2) shear modulus, 400 °C; (b3) shear modulus, 850 °C; (c1) bulk modulus, 10 °C; (c2) bulk modulus, 400 °C; (c3) bulk modulus, 850 °C.

![Figure 5](image2.png)

**Figure 5.** Temperature dependences of the maximum modulus (a) and minimum modulus (b) in the single-crystalline Ni$_3$Al.
Table 1. The maximum and minimum values of Young’s modulus, shear modulus, and bulk modulus in the single-crystalline Ni3Al at 10 °C, 400 °C and 850 °C.

| Modulus            | Maximum value (GPa) | Minimum value (GPa) | Temperature (°C) |
|--------------------|---------------------|---------------------|------------------|
| Young’s modulus    |                     |                     |                  |
| 270.0              | 108.2               | 10                  |
| 246.9              | 96.1                | 400                 |
| 214.0              | 80.3                | 850                 |
| Shear modulus      |                     |                     |                  |
| 121.5              | 40.3                | 10                  |
| 110.9              | 35.6                | 400                 |
| 95.7               | 29.6                | 850                 |
| Bulk modulus       |                     |                     |                  |
| 347.5              | 347.5               | 10                  |
| 319.3              | 319.3               | 400                 |
| 280.6              | 280.6               | 850                 |

4. Summary
To investigate the stress and strain concentration induced by different states of crystal orientations between the single-crystalline and polycrystalline Ni3Al under different temperatures, in this study, the mechanical properties of both single-crystalline and polycrystalline Ni3Al were evaluated and the influence of temperature on them were revealed. The Young’s modulus, shear modulus and bulk modulus of polycrystalline Ni3Al decrease linearly with the increase of temperature, and the relations between these moduli and temperatures have been established. Increasing temperature increases the universal anisotropy index of the single-crystalline Ni3Al. The bulk modulus of single-crystalline Ni3Al is isotropic. However, the Young’s modulus and shear modulus are obvious anisotropic, and their anisotropic characteristics are opposite. The increasing temperature decreases both maximum and minimum values of Young’s modulus, shear modulus, and bulk modulus of single-crystalline Ni3Al.

5. References
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