The elastic, strength and thermophysical characteristics modeling of mono- and polycrystalline aluminum Al

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Abstract. Temperature dependences of mechanical and thermophysical properties of the material are the initial data for estimating the stress-strain state of structural elements. However, when designing, the amount of this data is usually not enough. Under these conditions, the problem of modeling these properties arises. This problem is solved by taking into account the forces of interatomic interaction in the crystal structure on the example of a single crystal and polycrystal of aluminum. The results of calculating the elastic modulus, elastic limit and yield strength, Poisson's ratio, coefficients of thermal conductivity, thermal expansion and material density are presented. A satisfactory convergence with the available reference data is obtained. The results obtained can be used as input data for the construction of compositions and alloys based on aluminum.

1. Introduction

To assess the strength of the part material, it is necessary to know its temperature dependences of mechanical and thermophysical properties. In the case when there is not enough reference data, it becomes necessary to model them. In this paper the problem of modeling material characteristics is solved by taking into account the forces of interatomic interaction in the crystal structure.

2. Assumptions and calculation formulas

Assumptions

1. An elementary atomic cell of a defect-free single crystal with a lattice period of $a_0$ is considered.

2. The most closely packed planes of a single atomic cell of a single crystal and the crystallographic directions corresponding to these planes are considered. In particular, for a cubic lattice, planes and directions are shown in Figure 1. Thus, the anisotropy of the properties of a elementary atomic cell of a single crystal is taken into account.

3. Due to the symmetry of the crystal structure, the properties of an elementary atomic cell are transmitted to the macro volume of a single crystal.

4. The stress-strain diagram of a defect-free single crystal is characterized by a so-called "yield tooth" (figure 2, a). The stress-strain diagram model is shown in figure 2, b.
Figure 1. Directions and planes of the crystal lattice.

| a) experiment [1]; b) calculation model; 1-2-3-single crystal; 3-4-5-polycrystal |
|------------------|------------------|

Figure 2. Stress-strain Diagram of filamentous single crystal

In particular, the elastic characteristics of a single crystal are determined by the elastic modulus and the elastic limit (point 2 in figure 2, b). At that, the elastic limit exceeds the yield strength. Therefore, to calculate the yield strength of a single crystal, it is necessary to know the value of the elastic limit.

Due to the limited volume of the article, only some basic formulas are given here. The rest of the formulas can be found in the work [2].

The tangential component of the elastic limit for shear in a single atomic cell of a single crystal is calculated by the theoretical formula [1]

$$\tau = \frac{\varepsilon^2}{(d_0^2 \pi \varepsilon_0 A)} \left(1 - \cos^2 \gamma_{\text{max}}\right) \cos \left(\frac{\pi}{2} - \gamma_{\text{max}}\right)$$

where $\gamma$ - maximum shear angle corresponding to the elastic limit; $A$ - shear area; $\varepsilon = 1.6 \cdot 10^{-19}$, $C$ - the value of interacting charges equal to the electron charge; $\pi = 3.14$; $\varepsilon_0 = 8.85 \cdot 10^{-12}$, $C^2/Nm^2$ - electric constant; $d_0$ - the period of the crystal lattice.

The tensile yield strength of a single crystal is calculated by the theoretical formula [1]. It is based on the mechanism of displacement edge dislocation and the electrostatic nature of interatomic interaction

$$\tau = \frac{c}{\left(\frac{\pi}{2}\right)^2}.$$
where \( c \) - coefficient determined at the point \([\tau_{\text{max}}; x / a_0]\); \( x \) - the amount of displacement in an elementary atomic cell.

The relationship between the normal and tangential projections of the shear stress of a defect-free single crystal is determined by the formula [1]

\[
\sigma = \frac{\tau}{(\cos \alpha \cos \beta)}
\]  

(3)

where \( \alpha \) - is the angle between the horizontal plane and the shift plane; \( \beta \) - the angle between the shear plane and the direction of normal stress.

The change in the period of the crystal lattice due to an increase in temperature is calculated based on the change in the binding energy of two opposite charges in the crystal lattice. The dependence of the change in the period of the crystal lattice on the temperature is calculated using the theoretical formula [1]

\[
\Delta a_0 = 0.5 \left( \frac{c'v^2}{a_0} - c'_v \Delta T 2 \pi \varepsilon_0 \right)
\]  

(4)

where \( \Delta a_0 \) - change in the period of the crystal lattice due to thermal action; \( \Delta T \) – temperature change; \( c'_v \) – the heat capacity of the atom at a constant volume.

The formula for calculating the density of a single crystal of a simple substance consisting of atoms of a single chemical element has the form [2]

\[
\rho = \frac{m_A \cdot M \cdot k_p}{a_0^3}
\]  

(5)

where \( m_A \) is the atomic mass of the element; \( M = 1.66 \cdot 10^{-27} \) is the atomic unit of mass; \( k_p \) is the reticular density coefficient for an elementary atomic cell.

3. The results of calculation and comparative analysis

Figures 3-7 and tables 1-5 show the results of calculations and comparison with reference data of the following characteristics of mono- and polycrystal aluminum: elastic modulus, elastic limit and yield strength, Poisson's ratio, thermal conductivity ratio, thermal expansion ratio, density of the material.

Figure 3, a shows the temperature dependences of the elastic modulus, taking into account the anisotropy of the properties of the Al single crystal, in the crystallographic directions \( \langle 100 \rangle \), \( \langle 110 \rangle \), \( \langle 111 \rangle \). In figure 3, b - for a Al polycrystal in comparison with reference data (points on the graph) [3].
The coefficients of transverse strain (Poisson's ratio) \( \nu_{xy} \), \( \nu_{xz} \), are determined for uniaxial tension along the x axis (figure 1). If in an elementary atomic cell the x coordinate axis is combined with the direction \( \langle 100 \rangle \), then there is an "orthogonal isotropy", in other words, the elastic characteristics along the x, y, and z coordinate axes are the same. In this case, the Poisson's ratio is determined by the work formula [2]. If in an elementary atomic cell the x coordinate axis is combined with the direction \( \langle 110 \rangle \) or \( \langle 111 \rangle \), then anisotropy occurs. The calculation results are shown in table 1.

**Table 1. Poisson's Ratio**

| Parameter designation | The value of the parameter when the X axis coincides with the direction |
|-----------------------|-----------------------------------------------------------|
| \( \nu_{xy} \)         | (100) 0.352, (110) 0.192, (111) 0.477          |
| \( \nu_{xz} \)         | (100) 0.352, (110) 0.462, (111) 0.149          |

Figure 4, a shows the temperature dependences of the thermal expansion coefficient of the Al single crystal in the directions \( \langle 100 \rangle \), \( \langle 110 \rangle \), \( \langle 111 \rangle \). In figure 4, b - for a polycrystal in comparison with reference data (points on the graph) [3].

![Figure 4](image)

**Figure 4.** Temperature dependences of the coefficient of thermal expansion

The temperature dependences of the elastic limit (upper notation 100,110,111) and yield strength (lower notation 100,110,111) are shown in figure 5,a. In figure 5, b is the yield strength for a polycrystal in comparison with reference data (points on the graph) [4].

![Figure 5](image)

**Figure 5.** Elastic limit and yield strength of Al.
Figure 5. a shows that the maximum value of the elastic limit corresponds to the crystallographic direction \langle111\rangle. In turn, the maximum value of the yield strength point corresponds to the crystallographic direction \langle100\rangle. In particular, since the "stress-strain" diagram of a single crystal has a "yield tooth" (figure 2.a), the maximum value of the yield point is determined by the elastic limit. This information may be necessary for the development (construction) of single-crystal aluminum alloys.

Table 2. The yield strength

| Element designation | \(\sigma_{T100}\) (MPa) | \(\sigma_{T110}\) (MPa) | \(\sigma_{T111}\) (MPa) | \(\sigma_{T\text{ middle}}\) (MPa) | \(\sigma_{T\text{ ref}}\) (MPa) | \(\Delta\) % |
|---------------------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|
| Al                  | 48              | 17.6            | 28.8            | 31.5            | 30              | 32 [4]; 32 [5] ≈ ±1.5 |

Table 3. The propagation velocity of oscillations

| Element designation | \(v_{100}\) (ms\(^{-1}\)) | \(v_{1}\) (ms\(^{-1}\)) | \(v_{110}\) (ms\(^{-1}\)) | \(v_{111}\) (ms\(^{-1}\)) | \(v_{2}\) (ms\(^{-1}\)) |
|---------------------|-----------------|-----------------|-----------------|-----------------|-----------------|
| Al                  | 3534            | 3080            | 4997            | 5080            | 6123            | 6260            |

Table 3 shows that there is a satisfactory convergence between the values: \(v_{100}\) and \(v_{1}\), \(v_{110}\) and \(v_{2}\), \(v_{111}\) and \(v_{2}\). In particular, for aluminum, \(v_{110} = 4997\) m/s and \(v_{1} = 5080\) m/s, \(v_{111} = 6123\) m/s and \(v_{2} = 6260\) m/s.

The results of calculating the thermal conductivity coefficient are summarized in table 4.

Table 4. The thermal conductivity.

| Element designation | \(\lambda_{100}\) (Wm\(^{-1}\)K\(^{-1}\)) | \(\lambda_{110}\) (Wm\(^{-1}\)K\(^{-1}\)) | \(\lambda_{111}\) (Wm\(^{-1}\)K\(^{-1}\)) | \(\lambda_{\text{middle}}\) (Wm\(^{-1}\)K\(^{-1}\)) | \(\lambda_{\text{ref}}\) (Wm\(^{-1}\)K\(^{-1}\)) | \(\Delta\) % |
|---------------------|-----------------|-----------------|-----------------|-----------------|-----------------|---------|
| Al                  | 368.6           | 488.3           | 359.3           | 405.4           | 401             | 1.1     |

The average value values for a single crystal \(\lambda_{\text{middle}} = (\lambda_{100} + \lambda_{110} + \lambda_{111})/3\), is used as the thermal conductivity coefficient for a polycrystalline state. Table 4 shows that the calculation results satisfactorily converge with the experimental values for a polycrystal from the lsr reference literature [5] with a discrepancy of 1.3 %. These results also indirectly confirm the adequacy of the model for determining the rate of oscillations propagation velocity (table 4).

The results of calculating the temperature dependence of the crystal lattice period and the density of the Al polycrystal are shown in figures 6.7 in comparison with the reference data (points on the graph) [3,4].

![Figure 6](image6.png)  ![Figure 7](image7.png)
The density of Al as a function of temperature is also shown in table 5.

| Element designation | Density ρ, kg / m3 at temperature, C |
|---------------------|-------------------------------------|
| Al                  | 20  2699  100  2697  200  2687  300  2669  400  2643  500  2609  600  2586 |

Thus, the satisfactory convergence of the calculation results with reference data confirms the adequacy of the model, and also allows you to fill in the missing experimental data with calculated values.

4. Conclusion

1. The Developed model allows to Supplement the missing volume of reference data on elastic, strength, thermal and physical characteristics of the material.
2. The Model allows you to get the necessary information in conditions when the experiment is difficult to conduct for technical reasons, for example, at high temperatures.
3. The calculation results satisfactorily agree with the reference data for polycrystalline condition of the aluminum. In the case where reference information about the properties of a single crystal is available, there is also a satisfactory convergence, in particular for the elastic modulus of aluminum.
4. Calculations make up for the lack of reference information for the single-crystal state of aluminum on its elastic, strength and thermal characteristics, taking into account anisotropy, as well as depending on temperature.
5. The Results obtained are the initial data for the construction of compositions and alloys based on aluminum.

References

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