

# Eutectic composite NiAl-Cr properties modeling based on interatomic interaction forces

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**Abstract.** For new materials, information on the elasticity and strength characteristics necessary for calculating the stress-strain state of the turbine blades is limited. In these conditions, there is a need for theoretical methods for calculating the elastic and strength characteristics. The proposed theoretical methods are based on forces of interatomic interaction calculation. The classical methods based on the hypothesis of continuity do not allow calculating the material strength and thermophysical properties.

## 1. Introduction

The existing methods of calculating the strength of structural elements are based on the theory of the mechanics of a deformable solid body elasticity, which in turn is based on the hypothesis of continuity and empirical initial data.

Studies in the field of solid state physics have shown that the strength of solid bodies is based on the balance of the interatomic forces of attraction and repulsion between the crystal lattice sites. The application of this fundamental materials property makes it possible to develop methods for calculating the structural strength and proceeding to models of the materials behavior from the hypothesis of continuity to the forces of interatomic interaction calculation at the level of an elementary atomic cell. This approach opens the possibility of calculating theoretically the strength, elasticity and thermophysical characteristics of structural elements, which include: the modulus of elasticity, the Poisson's ratio, the elastic limit, the yield strength, the coefficient of thermal expansion, the coefficient of thermal conductivity, the density, which are the initial data in the calculation of the structural detail stress-strain state [1],[2].

Application of the developed model for a new alloy with a chemical composition determined by the regression analysis method allows reducing the volume of experiments and the duration of testing of these characteristics".

The problem is solved using the example of perspective eutectic composite type NiAl-Cr with a doped matrix based on nickel aluminide. This material has a higher heat resistance and lower density compared with high-temperature alloys on a nickel base. At the same time, their high-temperature strength characteristics are comparable.



## 2. The calculation model

Elastic modulus  $E$  is calculated for elementary atomic cell by the theoretical formula [1][2], based on the electrostatic nature of elasticity and derived from Coulomb and Hooke's law:

$$E = \frac{e^2}{4\pi\epsilon_0 r^2 a_0^2}, \quad (1)$$

where  $e = 1,6 \cdot 10^{-19}$ , C - the value of interacting charges equal to the electron charge;  $\pi = 3,14$ ;  $\epsilon_0 = 8,85 \cdot 10^{-12}$ , C<sup>2</sup>/N·m<sup>2</sup> - electric constant;  $a_0$  - the period of the crystal lattice;  $r$  - the distance between the interacting charges (depending on  $a_0$  and crystallographic direction).

The tangential component of the shift elastic limit in the elementary atomic cell single crystal is calculated by theoretical formula [1][2].

$$\tau_{\max} = \frac{e^2}{A\pi\epsilon_0 a_0^2} (1 - \cos^2 \gamma_{\max}) \cos\left(\frac{\pi}{2} - \gamma_{\max}\right), \quad (2)$$

where  $\gamma_{\max}$  - the maximum displacement angle corresponding to the elastic limit;  $A$  - shift area.

Tensile yield strength of the single crystal is calculated by the theoretical formula [1][2], based on the movement mechanism of an edge dislocation and the electrostatic nature of the interatomic interaction:

$$\tau = \frac{c}{\left(\frac{x}{a_0}\right)^2}, \quad (3)$$

where  $c$  - coefficient determined at point [ $\tau_{\max}$ ;  $x/a_0$ ];  $x$  - the amount of movement in the elementary atomic cell shift.

The thermal expansion coefficient is calculated in the following sequence. Initially the authors calculated change in the lattice parameter due to temperature increase, which calculation is based on changing the energy coupling of two opposite charges in the lattice. Dependence of the lattice parameter on the temperature calculated by the theoretical formula [1][2] is:

$$\Delta a_0 = 0.5 \left( \frac{e^2}{\frac{e^2}{a_0} - c_v^1 \Delta T 2\pi\epsilon_0} - a_0 \right), \quad (4)$$

where  $\Delta a_0$  - change in the period of the crystal lattice due to thermal effects;  $c_v^1$  - the heat capacity of an atom at a constant volume;  $\Delta T$  - temperature change.

For the atomic unit cell of the crystal lattice, thermal expansion coefficient  $\alpha$  is defined as [1][2]:

$$\alpha = \frac{\Delta a_0}{a_0 \Delta T}. \quad (5)$$

Density  $\rho$  of single crystals of simple substances is calculated by theoretical formula [1][2]:

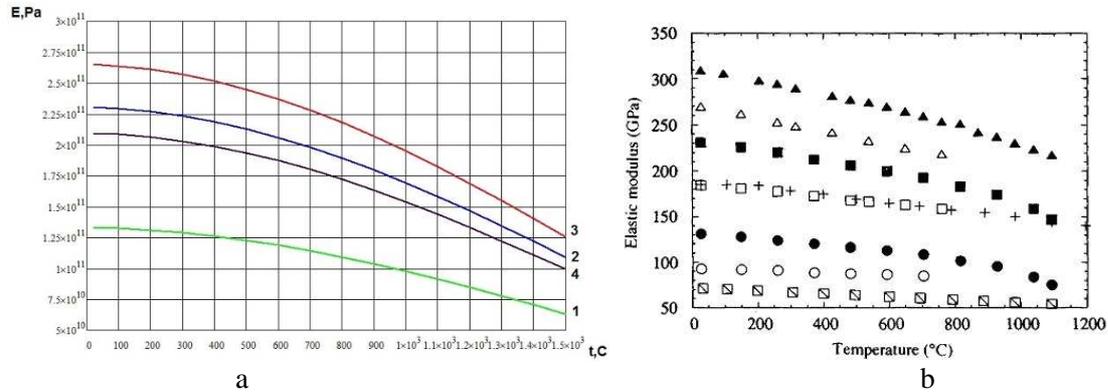
$$\rho = \frac{m_A k_p M}{a_0^3}, \quad (6)$$

where  $m_A$  - atomic weight of a chemical element;  $k_p$  - coefficient of the reticular density of the crystal structure unit cell;  $M = 1,66 \cdot 10^{-27}$ , kg - the atomic mass unit.

## 3. Initial data for composite components NiAl- Cr

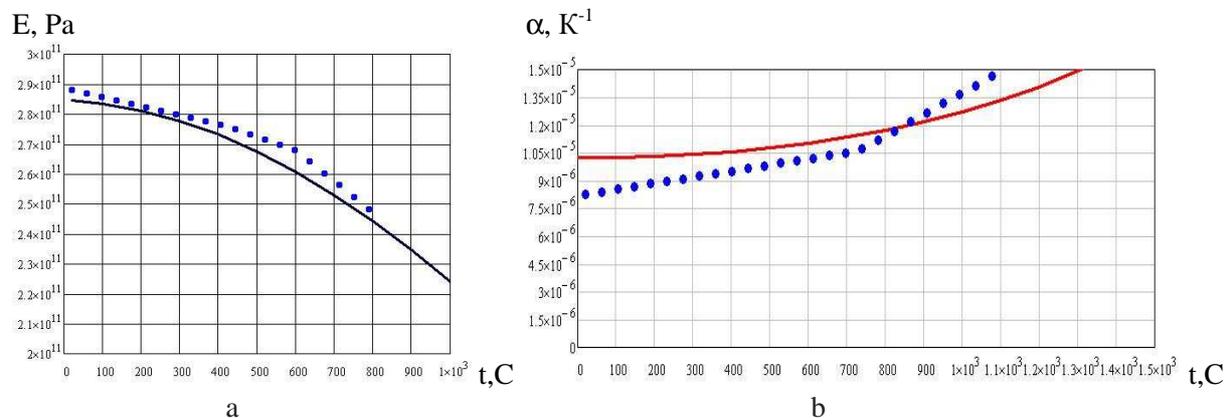
The main components of the eutectic composite are nickel-alumina matrix NiAl, the reinforcing phase is chromium Cr. To calculate the elastic and thermophysical characteristics, it is necessary to have temperature dependences.

The temperature dependences of the elasticity modulus of a nickel aluminide single crystal in crystallographic directions  $\langle 100 \rangle$ ,  $\langle 110 \rangle$   $\langle 111 \rangle$  and a polycrystalline are shown in Fig.1.



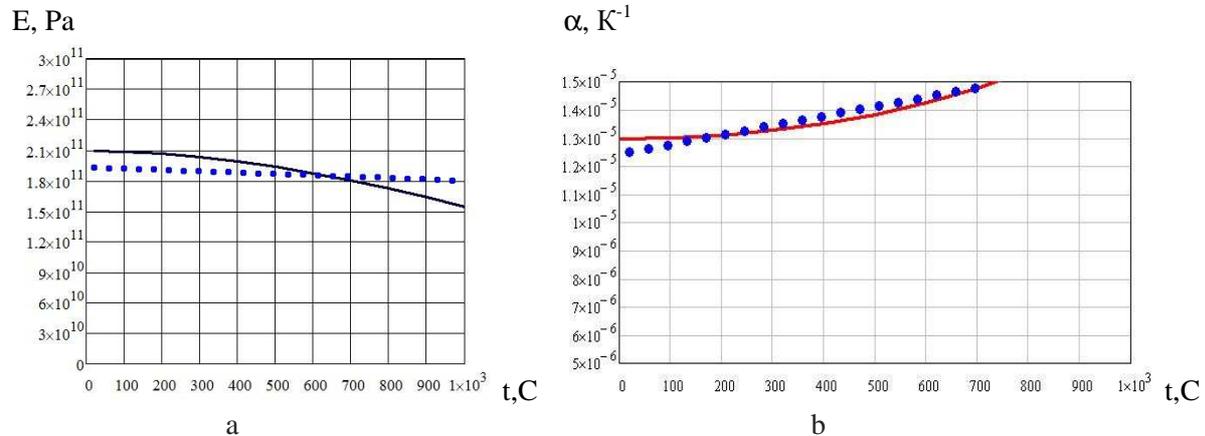
**Figure 1.** Temperature dependence of the elasticity modulus: a - nickel aluminide single crystal in crystallographic directions: 1 -  $\langle 100 \rangle$ , 2 -  $\langle 110 \rangle$ , 3 -  $\langle 111 \rangle$ , 4 - polycrystalline – calculation; b - reference data [3]: Young’s modulus as a function of temperature for single-crystal NiAl along the  $\langle 100 \rangle$  ( $\circ$ ),  $\langle 110 \rangle$  ( $\square$ ), and  $\langle 111 \rangle$  ( $\Delta$ ) directions (Wasilewski, 1966), and for single-crystal, Ni-based superalloy along the  $\langle 100 \rangle$  ( $\bullet$ ),  $\langle 110 \rangle$  ( $\blacksquare$ ) and  $\langle 111 \rangle$  ( $\blacktriangle$ ) directions (Lahrman and Darolia, 1992). The Young’s modulus (+) and shear modulus ( $\boxtimes$ ) of polycrystalline NiAl are also provided (Moose, 1991)

Fig. 2 shows the results of calculating the temperature dependences for polycrystalline Cr chromium in comparison with the reference data [4], [5].



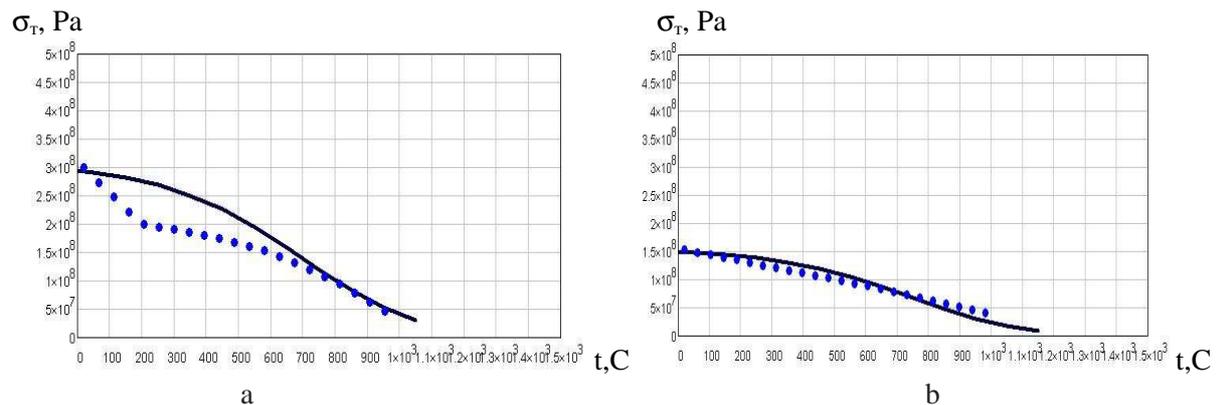
**Figure 2.** Temperature dependence: a - the elasticity modulus; b - the thermal expansion coefficient of the polycrystalline Cr ( — - calculation; ..... - reference data).

Fig. 3 shows the temperature dependences of the modulus of elasticity and the coefficient of thermal expansion for polycrystalline nickel aluminide NiAl.



**Figure 3.** Temperature dependence: a - the elasticity modulus; b - the thermal expansion coefficient of the polycrystalline NiAl (\_\_\_\_ - calculation; ... - reference data).

Fig. 4 shows the semi empirical temperature dependences of the yield stress for polycrystalline Cr and NiAl.



**Figure 4.** Temperature dependence of the tensile yield strength of polycrystalline: a - Cr; b - NiAl (\_\_\_\_ - calculation; ..... - reference data).

Fig. 1-4 demonstrate that the results of the calculation agree satisfactorily with the reference data [4][5]. It should be noted that for some elements and compounds reference data are available only for the polycrystalline state.

#### 4. Initial data for the composite

The characteristics of the composite are calculated according to the additivity rule (the blending method). The results of the calculation are obtained: elastic modulus  $E$ , shear modulus  $G$ , thermal expansion coefficient  $\alpha$ , thermal conductivity coefficient  $\lambda$ , density  $\rho$  as a function of volume fraction  $\psi$  of the fiber (reinforcing phase) in the matrix.

In particular, the density of the composition  $\rho_{cm}$  according to the mixture method is determined by the formula:

$$\rho_{cm} = \rho_f \psi + \rho_m (1 - \psi),$$

where the subscripts are  $f$  - fiber;  $m$  is the matrix;  $cm$  - composite material. The design density of the NiAl-Cr eutectic composite with a volume fraction of 30% reinforcing phase is  $6278 \text{ kg/m}^3$ .

It should be noted that when using a doped matrix based on nickel aluminide, the properties shown in Fig. 1-4 will change since the phase composition of the matrix (the base) is formed. Therefore, for the correct construction of temperature dependences, it is necessary to take into account the temperature at which the phases begin to dissolve. In this case, it is required to recalculate the stress-

strain state rotor blade.

### **5. The rotor turbine blade results of static strength calculation**

The obtained results of the elastic, strength, thermophysical and physical characteristics of the eutectic composite calculation make it possible to generate initial data for the thermal strength analysis of a turbine rotor blade made of a NiAl-Cr composite with orthotropic properties. Elastic stress-strain state calculation by the finite element method uses the typical temperature distribution in the longitudinal and transverse directions along the thickness of the pen of an uncooled blade. The given three-dimensional geometry of the blade, finite element grid, boundary conditions and loads is due to inertial and gas forces.

It was found that at the same points, the maximum stress at the leading edge of the NiAl-Cr blade decreased by approximately 28% compared to the starting material.

It should be noted that the long-term strength and, accordingly, the resource depend on the nature and the degree of doping of the matrix based on nickel aluminide [3].

### **6. Conclusion**

1. Application of the developed model allows one to reduce the volume of experiments and the duration of verification of the material characteristics at the stage of experimental determination of its service properties.

2. A calculated evaluation of the properties of the NiAl-Cr eutectic composite showed the possibility of reducing the weight of one blade by about 28%.

3. A calculated evaluation of the life of the long-term static strength showed its significant increase for a particular type of engine.

### **References**

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