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RELATION BETWEEN ELASTIC AND THERMAL PROPERTIES OF SINGLE CRYSTALS
OF HEAT-RESISTANT ALLOYS

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Elastic properties of single crystal samples of 60N21 steel and of some the heat-resistant nickel-based alloys differing by a volume fraction of strengthening γ' -phase are investigated, including niobium-doped Ni_3Al alloy. Elastic wave velocities are measured and components of elastic moduli tensor are determined. Debye temperature is calculated. Values of elastic anisotropy factor are determined.

Development of modern techniques needs creation of heat-resistant single crystal materials. Among them the greatest prospects have steel monocrystals, and also alloys on nickel basis. Heat-resistant nickel alloys are applied to blade manufacturing in stationary and aviation gas-turbine engines. They work in conditions of heats and in excited environments [1,2]. For this group of alloys the Ni_3Al intermetallic compound is base in which there are temperature anomalies of deformation characteristics, and also the effect of thermal hardening connected to them. It is known, that high elastic anisotropy renders the most essential influence on temperature dependence of ultimate strength [3]. Therefore a lot of experimental works has been devoted to measurement of elastic moduli of Ni_3Al single crystals in a wide temperature interval [3-6]. The ratio of the bulk modulus B to the Young modulus E can be considered as an authentic parameter of tendency of a material to fragile destruction. Measurements of the modulus B and analysis of the elastic anisotropy factor A are carried out in [5] with the purpose to find out the reason of abnormal temperature variation of strength.

Steel monocrystals also represent perspective object of research of elastic properties [7]. By present time only individual works by definition of elasticity moduli of steel single crystals are executed by ultrasonic methods [8,9]. At the same time studying of moduli and other physical characteristics has the practical importance [7]. Single crystals 60H21 could be considered as convenient modelling object. Their elastic properties were studied in [10,11], and the special attention was given to kind of acoustic fields in various structural conditions. In the given work comparison elastic and thermal characteristics of 60N21 steel is carried out.

Besides researches are lead on single crystal samples of $\text{Ni}_3(\text{Al-Nb})$ alloy and of some heat-resistant nickel alloys. In the first case samples were single-phase (γ' -phase), in the second case they were two-phase alloys (γ solid solution on the basis of nickel and intermetallic γ' -phase). The volume fraction of intermetallic phase varied in the investigated alloys over a wide range. Measurements of elastic wave velocities in several crystallographic directions are carried out. The components of elasticity moduli tensor are designed on the velocity values. Further the shear modulus G and the bulk modulus B have been determined, and the factor of anisotropy A is designed. The Debye temperature that is the important parameter for estimation thermal properties of an alloy is calculated using known values of moduli. The purpose of research was not only reception of numerical values of these characteristics, but also comparison of these values to a fraction of strengthening γ' -phase.

At first let's consider characteristics of the samples used in the work. A steel single crystal with composition: C (0,59 %); Ni (20,9 %); Mn (0,57 %); Si (0,3 %) is grown by Bridgemen method. Length of the sample, that is a distance between two plane-parallel planes, a normal to which in limits $\pm 2^\circ$ coincided with a direction [110], is equal 0,788 sm.

The contents of γ' -phase in the investigated nickel alloys varied from 5 volume percent for alloy EI-437B up to 67 % for alloy ZhS-36. Alloy TsNK-8MP is assigned to corrosion-resistant. In an alloy of VKNA-type, developed in VIAM, the volume fraction of intermetallic phase is increased up to 95 %. In a single crystal sample of an alloy with composition 75 % Ni - 19 % Al - 6 % Nb a volume fraction of γ' -phase achieves practically 100 %. The single crystals of EI-437 and $\text{Ni}_3(\text{Al, Nb})$ are grown by authors of the given work from melt by Bridgemen-Stockbarger method. Single crystals

of alloys ZhS-36, TsNK-8MP and VKNA are received under production conditions on Open Society "A.Ljulka-Saturn", Moscow.

Deviation of normal to a sample plane from crystallographic axes $\langle 001 \rangle$, $\langle 110 \rangle$ or $\langle 111 \rangle$ did not exceed $1^0 - 3^0$. Thickness of samples made 4 - 10 mm. Ultrasonic measurements are executed by an echo-method. Measurements were made on shear waves with frequency of 5 MHz and on longitudinal waves with frequency of 5 and 15 MHz. The error of velocity measurement makes no more than 0,5 %. Two samples of each material have been investigated for alloys on a nickel basis. In one sample the propagation direction has been chosen along an axis $\langle 100 \rangle$, in the another along an axis $\langle 110 \rangle$ or $\langle 111 \rangle$. Measurements on shear waves at the propagation direction $\langle 110 \rangle$ are carried out for two eigenmodes. Polarization directions of these eigenmodes are $u // [100]$ and $u // [1\bar{1}0]$. Results of measurements are shown in Table 1. The values of velocities measured in km/s are collected in the Table 1. The propagation direction is specified by a wave vector q .

Table 1. Elastic wave velocities

Alloy	Longitudinal waves			Shear waves			
	$q // [100]$	$q // [110]$	$q // [111]$	$q // [100]$	$q // [110]$		$q // [111]$
					$u // [100]$	$u // [1\bar{1}0]$	
60N21		5,59			3,73	2,09	
EI-437B	5,45		6,50	3,84			2,93
TsNK-8MP casted	5,46	6,28		4,03	3,97	2,37	
TsNK-8MP annealed	5,48	6,30		3,94	4,03	2,35	
ZhS-36	5,36	6,18		3,88	3,78	2,29	
VKNA	5,08	6,04		3,75	3,78	2,21	
Ni ₃ (Nb, Al)	5,56	6,42		4,08	4,04	2,34	

On values of velocities it is possible to calculate components of elastic moduli tensor of single crystals [12]. For a propagation direction [100] connection of moduli with velocities of waves is expressed by formulas

$$\rho s_{L[100]}^2 = c_{11}; \quad \rho s_{T[100]}^2 = c_{44}, \quad (1a)$$

where ρ is the density, $s_{L[100]}$ and $s_{T[100]}$ the phase velocities of longitudinal (L) and shear (T) waves with a propagation direction [100]. For a propagation direction [111] the similar formulas look as follows

$$\rho s_{L[111]}^2 = 1/3(c_{11} + 2c_{12} + 4c_{44}); \quad \rho s_{T[111]}^2 = 1/3(c_{11} + c_{44} - 2c_{12}), \quad (1b)$$

where for velocities of waves similar designations are entered at propagation direction [111]. In a direction [110] two eigenmodes propagate and the formulas connecting moduli and velocities of waves may be written as

$$\rho s_{L[110]}^2 = 1/2(c_{11} + c_{12} + 2c_{44}); \quad \rho s_{T1[110]}^2 = c_{44}, \quad \rho s_{T2[110]}^2 = 1/2(c_{11} - c_{12}), \quad (1c)$$

where the shear wave with polarization along [100] is designated by index $T1$, and the wave with polarization along $[1\bar{1}0]$ by index $T2$. For calculation of the module c_{12} the following formulas were used

$$c_{12} = \rho (s_{L[110]}^2 - s_{T1[110]}^2 - s_{T2[110]}^2). \quad (2a)$$

$$c_{12} = \rho (s_{L[100]}^2 + s_{T[100]}^2 - 3s_{T[111]}^2). \quad (2b)$$

The results received for moduli are listed in Table 2. In the same place on the references for comparison the values of the elastic moduli components for the intermetallic compound Ni₃Al are shown.

Table 2. Elastic module, density and Debye temperature

Alloy	Elastic module, GN/m ²			Density, kg/m ³	Debye temperature, K
	<i>C</i> ₁₁	<i>C</i> ₁₂	<i>C</i> ₄₄		
60N21	172	102	110	7,9	428
EI-437B	234	149	116	7,87	465
TsNk-8MP casted	252	140	137	8,46	471
TsNk-8MP annealed	254	152	131	8,46	472
ZhS-36	249	152	130	8,65	447
VKNA	215	145	117	8,35	382
Ni ₃ (Nb, Al)	240	141	129	7,75	467
Ni ₃ Al	223 [3]	148 [3]	125 [3]	7,56	462 [5]

The Debye temperature T_D is entered as limiting frequency in an oscillation spectrum of a solid. The Debye temperature can be defined from the elastic module values [13] using a method offered by Leibfried. Within the framework of this method calculation T_D is conducted following to the formula

$$T_D = \frac{h}{k} \left(\frac{3N}{4\pi V} \right)^{1/3} \left(\frac{c_{11} - c_{44}}{\rho} \right)^{1/2} J, \tag{3}$$

where h is the Planck's constant, k the Boltzman constant, N/V - number of atoms in unit of volume, and quantity J could be calculated depending on parameters

$$C = \frac{c_{44}}{c_{11} - c_{44}} = \frac{A}{2}, \quad K = \frac{c_{12} + c_{44}}{c_{11} - c_{44}}. \tag{4}$$

Results of calculation of Debye temperature are presented in table 2. The attention that fact pays to itself, that the Debye temperature for VKNA single crystal is appreciably less then for other materials.

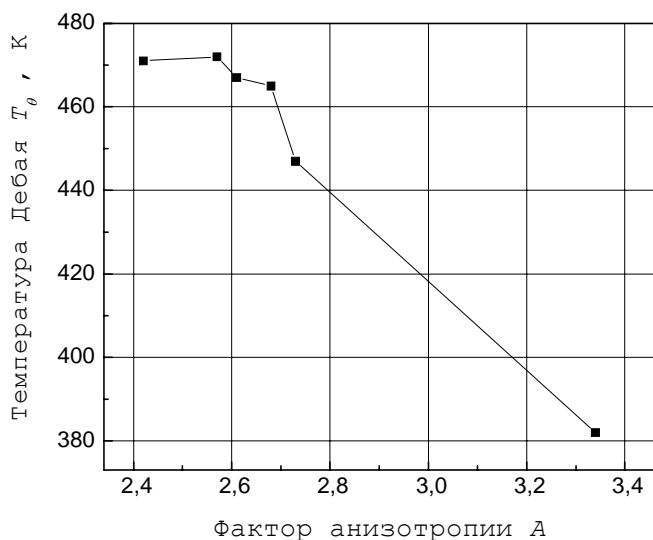


Fig.1. Correlation between the factor of elastic anisotropy and Debye temperature in heat - resistant alloys on a nickel basis

It is essential, that parameter C in the formula (4) is proportional to the factor of anisotropy A for a cubic crystal. Therefore, using method designed by Leibfried, it is possible to try to check up presence of correlation between elastic anisotropy and thermal characteristics of a material. About an opportunity of such correlation in heat - resistant alloys it was spoken in [3]. Results of calculation of the factor of anisotropy

A are shown in table 3. On Fig.1 alloys are located in ascending order the factor of anisotropy from cast TzNK-8MP with the least factor $A = 2,42$ up to alloy VKNA with very great value $A = 3,34$. On an ordinate axis in Fig.1 the values of Debye temperature are plotted. Distinct correlation is evident: with increase of anisotropy of a crystal the Debye temperature goes down. The value of the anisotropy factor A , certain by us for alloy BKHA, coincides with the value for Ni₃Al from [3]: $A=3,34$. From elastic moduli received the tensor components resulted in table 3, have been designed the bulk module B and the shear module G . For calculation relations are used

$$B = \frac{c_{11} + 2c_{12}}{3}, \quad G = \frac{G_V + G_R}{2}, \quad (7)$$

$$G_V = \frac{c_{11} - c_{12} + 3c_{44}}{5}, \quad G_R = \frac{5(c_{11} - c_{12})c_{44}}{4c_{44} + 3(c_{11} - c_{12})}$$

where an "isotropic" modulus G is introduced as average between modulus G_R (that is the bottom border of an estimation of modulus G) and modulus G_V (the top border of an estimation of modulus G). Results of calculations are shown in table 3.

Table 3. Elastic moduli B and G and anisotropy factor of alloys

Alloy	Anisotropy factor	Modulus B , GN/m ²	Modulus G_V , GN/m ²	Modulus G_R , GN/m ²	Modulus G , GN/m ²	Relation B/G
EI-437B	2,73	1,77	0,87	0,69	0,78	2,28
TzNK-8MP casted	2,42	1,77	1,05	0,87	0,96	1,85
ZhS-36	2,68	1,84	0,97	0,78	0,88	2,10
VKNA	3,34	1,68	0,84	0,60	0,74	2,27
Ni ₃ (Nb, Al)	2,61	1,74	0,97	0,79	0,88	1,98

In summary we shall note, that in this work velocities of elastic waves have been measured in a 60N21 steel single crystal and its elasticity tensor has been restored. The factor of anisotropy which appeared one of the biggest for cubic crystals of transition metals is determined. The Debye temperature values are determined. Acoustic research of elastic properties of some heat - resistant nickel alloys (EI-437B, TzNK8-MP, ZhS-36, VKNA) is carried out. Components of elastic moduli tensor are obtained. Values of the factor of anisotropy are determined and Debye temperature values are obtained by Leibfried method. There is a distinct correlation between the factor of anisotropy of a crystal and Debye temperature.

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