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A temperature change in elastic and acoustic properties of auricupride

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Abstract. Changes in acoustic and elastic properties of auricupride approach within the high temperature interval and close to an order-disorder phase transition have been discussed. Calculations of the phase velocities of purely transverse and longitudinal elastic waves, elastic moduli and Poisson's ratios based on elastic constants $c_{ij}(T)$ of the crystal have been executed. Temperature changes of Grüneisen parameter along crystallographic directions [100], [110] and [111] have been defined.

1. Introduction

Elastic properties of crystals are the most important properties of solids. The elastic properties of crystals are characterized by different modules and elastic constants adequately revealing the nature of interatomic bonds, which is one of the main problems of the solid state physics. The elastic properties anisotropy allows estimating on the interatomic bond strength in different crystalline planes.

Elastic properties and anharmonic effects in metallic, covalent, ionic, ion-covalent and molecular cubic single crystals with lattices of various types were studied in [1-3]. Anisotropy of elastic properties and anharmonicity of atomic interaction in the auricupride – binary alloy Cu_3Au with the positional order-disorder in the low-temperature region were considered in [4]. In the low temperatures area the given alloy has a cubic face-centered lattice with a $Pm\bar{3}m$ space group where face centers are occupied by copper atoms and cube corners by aurum atoms. A high-temperature disordered phase of Cu_3Au alloy is observed at the temperatures over $T_c = 661$ K. It has a face-centered cubic lattice where Cu and Au atoms are distributed in all positions without a long-range order. Elastic properties of a single crystalline alloy were studied by the method of a compound piezoelectric vibrator within the temperature range of 293…723 K (especially thoroughly near T_c) in [5].

2. Calculated ratios

Use the data on $c_{ij}(T)$ [5] of the auricupride crystal we have executed calculations of phase velocities of purely longitudinal and transverse bulk acoustic waves (BAW) in three crystallographic directions, elastic anisotropy factor (A), Cauchy relation (Δ) both for the ordered and disordered forms within a wide temperature range. The formulas for calculating phase velocities along directions [100], [110] and [111] are given in [4].

The stiffness constants were measured with the following inaccuracies: c_{11} – 0.8 %, c_{12} – 1.13 %, c_{44} – 0.23 %. According to these inaccuracies the maximal error of phase velocity determination in any direction does not exceed 0.5 %.

An elastic anisotropy factor determining the crystal isotropy measure was found according to ratio $A = 2c_{44}/c_{11} - c_{12}$ (for elastically isotropic body $A = 1$). Couchy relation which defines a measure of the central interatomic forces (under $\Delta = 1$ all interaction forces in the crystal must be central) equals to $\Delta = c_{12}/c_{44}$. The elastic properties of isotropic solids are characterized by elastic moduli B (bulk modulus of elasticity), E (Young modulus), G (shear modulus) and were found by the Voigt-Reuss-Hill (VRH) approximation (a cubic system) [4]. Elastic compliances s_{ij} were used for calculating the elastic moduli of the Cu_3Au alloy in the various crystallographic directions. The formulas for calculating the Poisson's ratio along three specific directions $\sigma_{\langle hkl \rangle}$ were presented in paper [6].

3. Results and discussion

Temperature changes of BAW phase velocities, elastic constants, etc. of the auricupride alloy within the interval of 300…725 K are linear both in the ordered and disordered phases with the exception of a narrow temperature interval near $T_c \approx 661$ K (Figures 1-3). Stiffness constants, phase velocities and elastic moduli do not decrease much with the temperature growth but Poisson's ratios demonstrate the tendency to an increase.

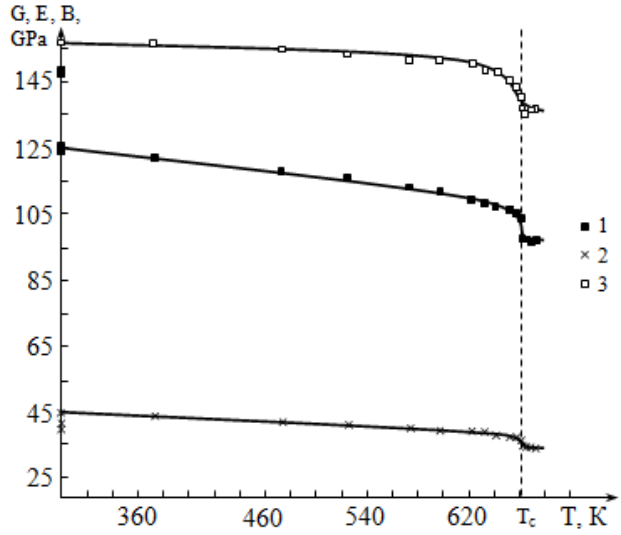

Figure 1. Change of elastic moduli of the auricupride polycrystal conditioned by temperature alteration: 1 – Young modulus E, 2 – shear modulus G, 3 – bulk modulus B.

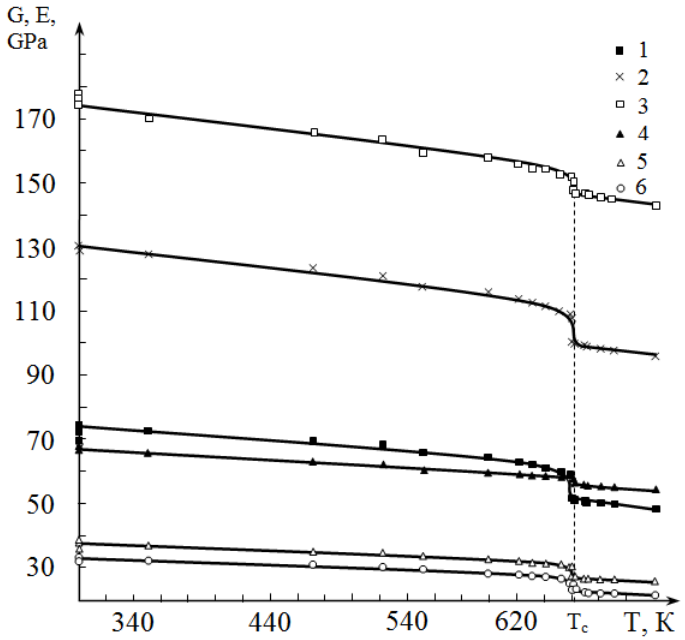

Figure 2. Change of elastic moduli of the auricupride monocrystal conditioned by temperature alteration in various crystallographic directions:
$1-\mathrm{E}_{\langle 100\rangle}$; $2-\mathrm{E}_{\langle 110\rangle}$; $3-E_{\langle 111\rangle}$; $4-\mathrm{G}_{\langle 100\rangle}$; $5-\mathrm{G}_{\langle 110\rangle}$; $6-\mathrm{G}_{\langle 111\rangle}$.

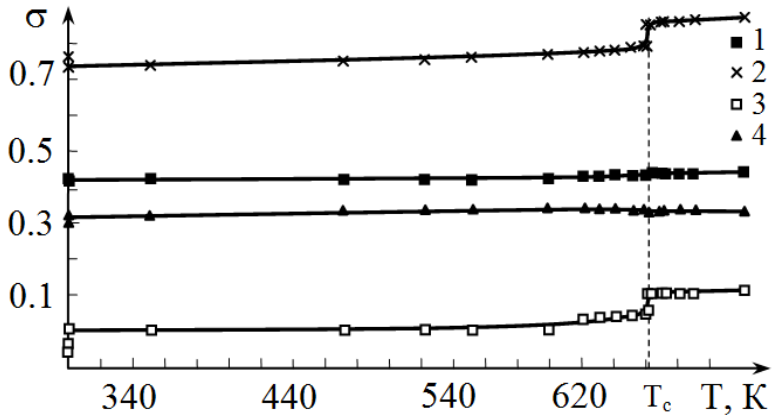

Figure 3. Change of Poisson's ratios monocrystal conditioned by temperature alteration in various crystallographic directions: $1-\langle 100\rangle$; $2-\langle 110,001\rangle$; $3-\langle 110,1\bar{1}0\rangle$; $4-\langle 111\rangle$.

From Figure 1 it is possible to see that all three effective elastic moduli (*G*, *E*, *B*) of auricupride near T_c demonstrate anomalous behavior ('softening' when a 'step' decreases by almost 10 %) which is associated with the phase transition into the disordered state.

Anisotropy of elastic properties of the auricupride alloy influences the relation between Young's and shear moduli in various crystallographic directions (Figure 2). Inequations between elasticity moduli for a given alloy are similar to the known dependencies between magnitudes $\mathrm{E}_{\langle hkl\rangle}$ and $\mathrm{G}_{\langle hkl\rangle}$ for the set of lithium halogenides under $A>1$: $\mathrm{E}_{\langle 111\rangle}>\mathrm{E}_{\langle 110\rangle}>\mathrm{E}_{\langle 100\rangle}$ and $\mathrm{G}_{\langle 100\rangle}>\mathrm{G}_{\langle 110\rangle}>\mathrm{G}_{\langle 111\rangle}$. Temperature changes of Poisson's ratios in the

auricupride alloy for various crystallographic directions are presented in Figure 3. In the temperature range from 300 to 725 K the following correlation is fulfilled: $\sigma_{\langle 110,001\rangle} > \sigma_{\langle 100\rangle} > \sigma_{\langle 111\rangle} > \sigma_{\langle 110,1\bar{1}0\rangle}$. Near T_c, Poisson's ratios increase abruptly (approximately by 10 %) under auricupride crystal deformation in two directions ($<100>$ and $<110,1\bar{1}0>$). The described peculiarities of acoustic and elastic properties near T_c demonstrate that the phase transition in auricupride is partly isothermal (a first-order phase transition) and partly smooth (a second-order phase transition).

4. Conclusion

We have applied the date on stiffness constants to calculated the BAW velocities along three special crystallographic directions of single crystalline alloy Cu_3Au. It has been established that among the longitudinal wave velocities $\upsilon_{L[111]}$ have the maximal value and the velocity of transverse waves is maximal in the [100] direction for all the temperature ranges. Temperature-related elastic moduli (Young, shear, bulk) changes are linear (the moduli decrease with the temperature growth with the exception of the temperature region near T_c). Thermal dependences of Poisson's ratios are also linear, although σ slightly increases with the temperature growth.

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