ON POSSIBILITY OF CU ELASTIC MODULI EVALUATION BY X-RAY DIFFRACTOMETRY DATA

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ABSTRACT

By using of lattice f.c.c. model with the central interaction in a first coordination sphere by known x-ray diffractometry data were evaluated Cu $C_{\mu\nu}$ elastic moduli in harmonic approximation. With accounting of conductivity electrons and zero oscillations influence on deviations from Cauchy correlations the results of calculations were appeared in reasonable correlation with existing experimental data.

KEYWORDS: *diffraction spectra, characteristic temperature, elastic modul*

INTRODUCTION AND THE SETTLEMENT OF PROBLEM

It is known, that from the intensities and x-ray interferentions shift thermal dependencies data may be obtained some information about dynamics of crystalline lattice: coefficients of thermal expansion α(T), the values of x-ray characteristic temperatures Θ(T) and their thermal dependencies $\Theta_p(T)$.
In work [1] was showed, that Θ_p is the characteristic of f-MΘ^2_p connection rigidity, at least at central interactions in first two coordination spheres. In one's turn, the $\Theta_p(T)$ dependence, actually, is reflecting decreasing of crystalline elastic moduli C_{ijkl} with growth of temperature and may be used for determination of Gruneisen parameters and force constants f,g,h, figurating in expansion of lattice potential by displacements ranges [2,3]. Further, using the f.c.c. lattice model with central interaction of nearest neighboures, one can evaluate the values of ant their thermal dependencies, if f,g,h are known [4]. Despite the circumstance, that such models leads to fulfilment of Cauchy's ratios $C_{ijkl} = C_{jikl}$ ($i \neq j$), they are elastically stable and in contrast to continual were characterized with dispersion of oscillations [4,5].
From this point of view may be interesting the using of the single parameter f, obtained from x-ray diffractometry data, to calculate values of Cu C_{ijkl} at T=0.The range of calculation reliability may be increased by taking to account further the influence of electrons of conductivity [6] and zero oscillations [7].In this work such calculation of C_{ijkl} is provided for Cu.The choice of Cu is caused by a reason, that for copper x-ray diffractometry Θ_p and $\Theta_p(T)$ data are most spreaded and correlating.

RESULTS OF CALCULATION AND DISCUSSION

According to [5] for f.c.c. lattice in harmonic approximation, elastic moduli in Foight signature ($C_{ijkl} \rightarrow C_{\mu\nu}$) correspondingly are equal to:

$$C_{11}=2f/a;\ C_{12}=f/a;\ C_{44}=f/a, \qquad (1)$$

where a – the lattice parameter, f – link rigidity parameter, determined as $f=0{,}15(k/\hbar)^2 m\theta^2_\rho(0)$ [3] (in standard signature).
At temperature T=0 parameter f, according to [3], may be determined as:

$$f = 0{,}1397\left(\frac{k}{\hbar}\right)^2 m\theta_\infty^2 \qquad (2)$$

For determination of harmonic values for $\tilde{f}$ and $C\tilde{\mu\nu}$ parameters one must use $\tilde{a}(0)$ and $\tilde{\Theta\rho}(0)$, quantities, which are

conditioned by the way of linear extrapolation of experimental dependencies *a*(T) and *θρ*(T) from a region of high temperatures T>θρ to T=0 K [4]. Such extrapolation is more rightful for θρ(T), than for θ_D(T), because a thermal dependence of the first of them actually is not influenced with low-thermal anomalies, conditioned by the difference of the real frequency spectral distribution function g(ω) from Debye parabola [3]. As showed in [2]

Θρ(T) = θρ(0) (1- 2γβ(T-T0)), (3)

where β - the volumetrical thermal expansion coefficient.

The necessary x-ray diffractometry data, obtained by calculations of C after (1) are adduced in table 1.

Table 1

metal	*θρ K*	γr	$\beta \cdot 10^6 K^{-1}$	*Θρ*(0)	*ã* (0)·10^{10}m	$f \cdot 10^4$ dyn/cm²
Cu	298	1,96	54,42	317	3,5940	2,763
C~μv · 10^{-12} dyn/cm ²						
C_{11}		C_{12}		C_{44}		
1,538		0,769		0,769		

Because for metals the Cauchy ratio is not accomplished, one may have a reason to take into account non-central interactions, using the known De-Launey model [6], according to which for metals of cubic symmetry

$$C_{12} - C_{44} = K_{el} \qquad (4)$$

where K_{el} - the pressing module of electron gase of conductivity. The value of K_{el} may be calculated by determination of Fermy energy μ_0 of collectivized electrons at T=0 K.

$$K_{ел} = 2/3\mu_0/V, \quad \text{де}$$

$$\mu_0 = \frac{h}{2m}\left(\frac{3Nn_0}{8\pi V}\right)^{\frac{2}{3}} \qquad (5)$$

From other side, even at T=0 K and central interactions the transgression of Cauchy relation is conditioned by the existence of zero oscillations, which in addition are unharmonic. This circumstance may be taking into account by using [4] (correlation 15.27)

$$C_{12} - C_{44} = \frac{9U(T)\gamma^2}{NV_Z} \qquad (6)$$

where N – Avogadro number; V- the volume of elementary cell; U(T) – the energy of lattice oscillation, which is equal to zero energy $U(0)=9/8 \cdot Nk\theta_D$ at T=0 in Debye approximation. Cause at T=0 the substitution has appears as a good approximation, the parameter in (5) one way take equal to ordinary Gruneisen parameter, given in table 1.

One may see from (4) and (6), that the influence of conductivity electrons and zero oscillations on declinations from Cauchy ratios requires the accounting of their summary deposition. The procedure of specification of adduced in table 1 values Cμυ for Cu is described below.

Using known numerical values of V_z, n_0, and m*, one can obtain μ_o=7,1eV, K_{el} = 0,769·10¹² dyn/cm². Further, taking to account (4) and (6), we have obtain:

$$C_{12} - C_{44} = 0{,}244 \cdot 10^{12} \text{ dyn/cm}^2. \qquad (7)$$

Using data of table 1 and follow (6) one may find: C_{12}=1,013·10¹² dyn/cm², C_{44}=0,769·10^{12} dyn/cm².

The self-coordination of results for such specified calculation of $C_\mu \nu$ may be easy verified by determining of Young and shift moduli E and G. Numerical values of elastic moduli , calculated with using of $C\mu\nu$, Cu, are given in table 2.

It is clear, that specified in a such way elastic moduli values for Cu must be compared with harmonic values $C_\mu \nu$(T) from a region of high temperatures at T= 0 K. A such comparison is reflected in a table 2, where $C_\mu \nu$ and elastic moduli Cu are taken from [7].

Table 2.

Determination	Cμυ GPa			Elastic moduli		
	C_{11}	C_{12}	C_{44}	*Ex.* GPa	*Gx.* GPa	K GPa
Calculation	153,8	101,3	76,9	123,4	50,7	118,8
Exper. extrapolation for T=0 [ ]	176,2	124,9	81,7	137,4	51,4	142,0

From a table one may see, that although the evaluation of $C_{\mu\upsilon}$ is made with using of simplified theoretical models, their results, nevertheless, are in reasonable correlation with experimental data for Cu and the maximal declination makes up about 10 %.
Let us note in conclusion, that the using of θρ as a measure of rigidity of (f~Mθ²ρ) connection , in combination with physical reasoning, described in [1], may be useful also in applied context. It is clear, that described above process of $C_{\mu\upsilon}$ evaluation by x-ray diffractometry data can not be regard as the universal method. Nevertheless, for such objects as alpha-solid solutions on a base of Cu, Ag et al metals with known electron concentration, such previous evaluations of $C_{\mu\upsilon}$, with no doubt may appeared useful.

CONCLUSIONS

1. There was showed the possibility of Cu elastic moduli evaluation by known x-ray diffractometry data with using of lattice f.c.c. model with central interaction.
2. There are obtained values of elastic moduli with accounting of electrons of conductivity and zero oscillations influence on deviations from Cauchy ratios, were appeared in reasonable correlation with experimental data.

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