T. I. Babjuck, Sc. (Eng.), Assist. Prof.; S. G. Avdejev, Assist. Prof.

USAGE OF X-RAY DIFFRACTOMETRY DATA FOR EVALUATION OF CU-BASED SOLID SOLUTIONS ELASTIC MODULES

Appling the model of face-centered cubic (f. c. c.) lattice with central interaction in the first coordinate sphere, by the known x-ray diffractometry data of elastic moduli $C_{\mu\nu}$ of Cu-Zn, Cu-Al and Cu-Sn solid solutions in harmonic approximation were evaluated. Obtained values of elastic moduli are compared with known published data.

Keywords: *diffraction spectra, elastic moduli, quasielastic force, characteristic temperature*

INTRODUCTION AND PROBLEM SETUP

It is known, that from the data of temperature dependence of intensities and x-ray interferences shift, certain information, regarding the dynamics of crystalline lattice, may be obtained: coefficients of thermal expansion $\alpha(T)$, values of x-ray characteristic temperatures Θ_p and their thermal dependencies $\Theta_p(T)$.

It was showed in [1], that Θ_p characterizes $f \sim M\Theta_p^2$ connection rigidity, at least at central interactions in the first two coordinate spheres. In its turn, the $\Theta_p(T)$ dependence, actually, reflects the decreasing of crystalline elastic modules C_{ijkl} with the growth of temperature and may be used for determination of Gruneisen parameters and force constants *f, g, h,* occurring in decomposition of lattice potential by displacements range [2, 3]. Further, using the face-centered cubic (f. c. c.) lattice model with central interactions of nearest neighbours, one can evaluate the values of C_{ijkl} and their thermal dependencies, if *f, g, h* are known [4]. For evaluation of this model application while study of α -solid solution Cu-Zn, Cu-Al, Cu-Sn properties it is quit interesting by available experimental x-ray diffractometric data evaluate elasticity modulii C_{ij} using the coefficients of quasielastic force of the indicated systems. It is quite obvious, that the model is too simplified for *Cu* and its solid solutions. Nevertheless, such a model is elastically stable [3] taking into account explicitly atomic structure, possesses the dispersion of thermal oscillations and hence, is more realistic, as compared with continual one. To some extent the error of such model in the process of *f* determination can be evaluated, comparing numerical values of *Cu* elasticity modules and some solid solutions, calculated by values of $C_{\mu\nu}$ with experimental data (see Table 2). Input data for calculation of Cu-Zn, Cu-Al, Cu-Sn parameters were X-ray characteristic temperatures Θ_p and their temperature dependences $\Theta_p(T)$ obtained from the analysis of temperature dependences of intensity and shift of X-ray interferences in wide temperature intervals [5 – 7].

RESULTS OF CALCULATIONS AND DISCUSSION

According to [8] for f. c. c. lattice in harmonic approximation, elastic modulii in Foight designations $(C_{ijkl} \rightarrow C_{\mu\nu})$ correspondingly equal to:

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

where α – is the lattice parameter, f – the link rigidity parameter.

At temperature $T=0$ parameter f, according to (3), is determined as

$$f= 0{,}1397\ (k/h)^2\, m\Theta_\infty^2 \qquad (2)$$

where k and h are Boltsmann and Plank constants, m – the mass, Θ – the characteristic temperature.

For determination of harmonic values for $\widetilde{f}$ and $\widetilde{C}_{\mu\nu}$ parameters one must use $\tilde{a}(0)$ and $\widetilde{\Theta}_p(0)$ quantities, obtained by means of linear extrapolation of experimental dependencies $\alpha(T)$ and $\Theta_p(T)$ from the region of high temperatures $T > \Theta_p$ to T=0 K [4]. Such extrapolation is more rightful for

Θ_p *(T)*, than for $\Theta_p(T)$ (calorimetric), because the thermal dependency of the first of them actually is not influenced by low-thermal anomalies, conditioned by the difference of the real function of spectral distribution $g(\omega)$ of frequencies on Debye parabola [3]. Numerical values of quasielastic force coefficient of Cu-Zn Cu-Al and Cu Sn systems solid solutions are presented in Table 1.

Table 1

VALUES OF COEFFICIENT *f* IN Cu-Zn, Cu-Al, Cu-Sn ALLOYS

№	Cont. of Zn in alloy, at. %	f 10 ^{4} erg/cm^2	Cont. of Al in alloy, at. %	f 10 ^{4} erg/cm^2	Cont. of Sn in alloy, at. %	f 10 ^{4} erg/cm^2
1	Cu(O)	2.370	0	2.37	0	2.37
2	4.50	1.82	0.98	2.35	2.70	2.68
3	9.40	1.50	4.80	2.81	4.80	2.56
4	18.48	1.38	6.80	1.70	6.50	2.39
5	20.85	1.22	11.25	1.65	8.90	2.26
6			12.85	1.68	11.03	2.12
7			15.35	1.76		

For evaluation of the third elastic component of cubic crystal transversal counteraction modules C_{12} we can use the relation, obtained in [9] (see p. 42) for cubic lattices:

$$C_{12}/C_{11} = 0.78 \qquad (3)$$

Using the values of quasielastic force coefficients *f* (Table 1), relations (1) and (3) isothermal elastic modules C_{11}, C_{12} and C_{44} , and also Young module E for some α -solid solutions of Cu-Sn system are determined. Concentration dependence for elastic module C_{11} of investigated systems is presented in Fig. 1.

One can see from Fig. 1, that with growth of soluted elements concentration in solid solutions the elastic module C_{11} decreases. The insignificant increasing of elastic module in the region of low concentrations (see Fig.1) may be explained by replacement of Cu atom with atoms of Zn, Al, Sn, their radii being larger, than the Cu one, that leads to local deformation of crystalline lattice. At least, in first two coordination spheres atoms of matrix are positioned closer to each other, than in underformed crystal. This circumstance leads to appearance of local pressure, which causes the increasing, according to (3,6) and (3,8), of [10] Debye's temperature and elastic module.

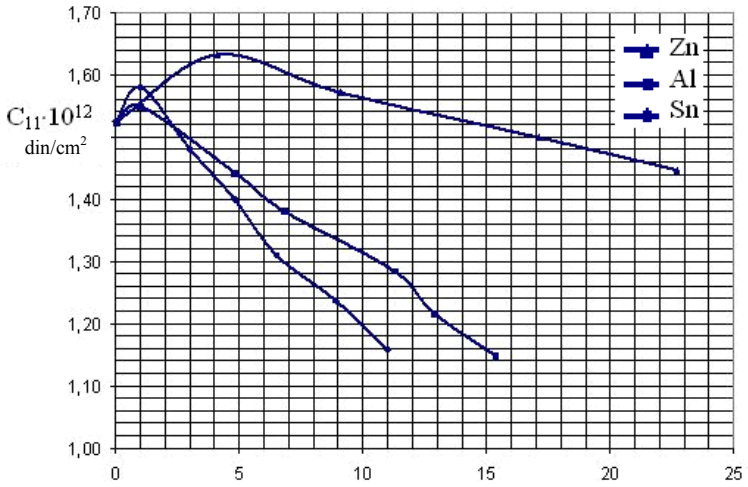

Fig. 1. Concentration dependencies of elastic module C11 for Cu-Zn, Cu-Al, Cu-Sn alloys. Content of Zn, Al Sn - in at. %

Moreover, in alloys of copper with metals of different valence the elastic module decreases with the growth of dope atomic concentration this growth is more visible, as higher the valence of doped

element (see Fig. 1). In these alloys introduced dope enlarges the electron concentration in the base metal lattice, and, therefore, increases the share of electron kinetic energy, which is accompanied by reduction of interatomic links and lowering of chemical strength. By the degree of influence on lowering of interatomic interaction in copper lattice dopes are arranged as Zn, Al, Sn.

Concentration dependence of elastic module C_{12} of α–solid solutions Cu-Zn, Cu-Al and Cu-Sn is presented in Fig. 2.

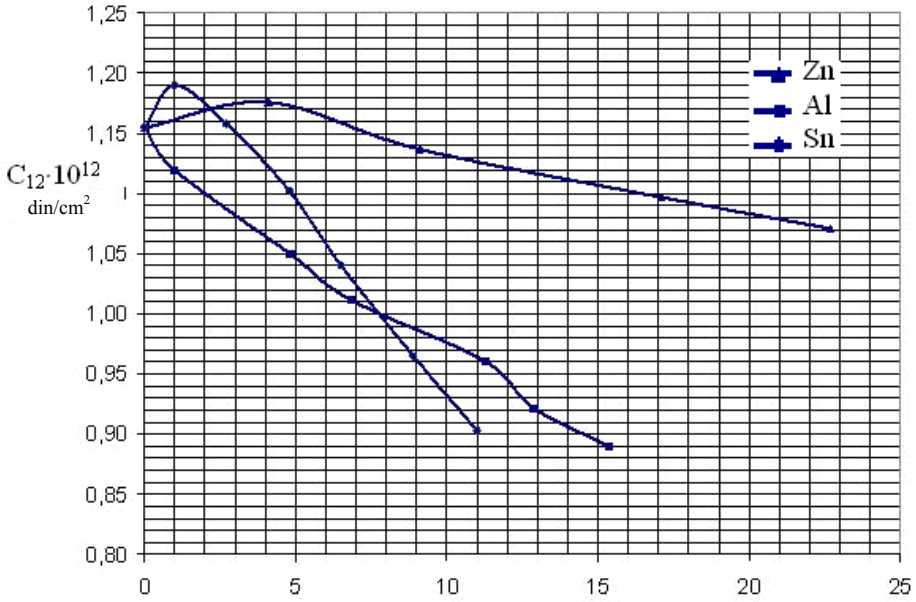

Fig. 2. Concentration dependence of elastic module C_{12} for alloys of Cu-Zn, Cu-Al, Cu-Sn. Content of Zn, Al, Sn in at. %

It is seen from Fig. 2, that the elastic module C_{12} with growth of concentration gradually decreases. With the accuracy of pattern scale this decreasing reflects the dependence of C_{12} module on concentration. The rate of $\partial C_{12}/\partial C$ change per one percent of concentration gives 0.14 as compared with 0.24 for C_{11}.

The dependence of elastic module C_{44} on different valence doping elements concentration in copper alloys is presented in Fig. 3.

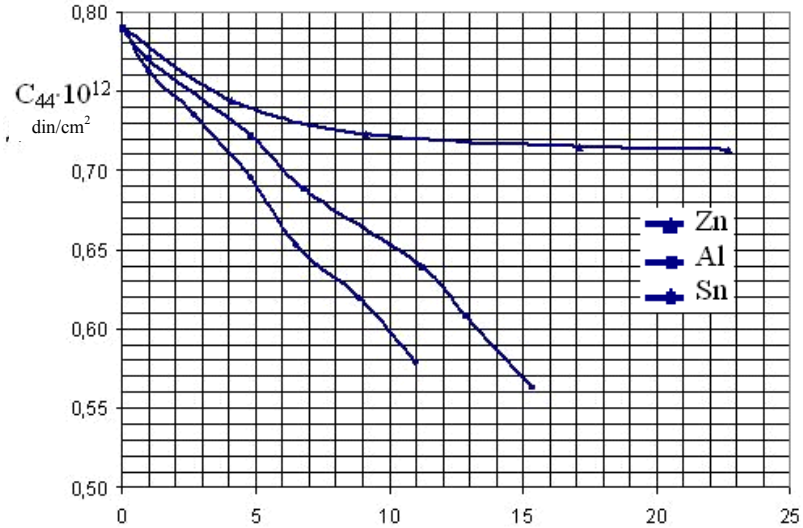

Fig. 3. Concentration dependence of elastic module C_{44} for Cu-Zn, Cu-Al and Cu-Sn alloys. The contents of Zn, Al, Cu - in at %

In the figure we can see, that substitution of Cu atoms by Zn atoms influences insignificantly on the elastic module C_{44} concentration dependence. It can be explained by the fact, that the valence and atomic radius of introduced dope in alloy have no significant difference between each other.

As Young module is the measure of the second derivative from the potential energy with the interatomic distance in crystalline lattice, it may serve as a measure of interatomic links strength in solid solution.

The numerical values of Young module E, calculated by C_{ij} ones of the noted solid solutions, are presented in Table 2.

For the comparison experimental values of Young module E_{exp} of some solid solutions of investigated systems taken from [9], are given in Table 2.

From the Table one can see, that, despite the fact, that evaluation of Cij values was carried on using simplified theoretical models, their results, nevertheless, in rational measures are correlated with the experimental data for a number of solid solutions and the maximal deviation is growing up to ~ 10 %.

Table 2

Values of Young module E for α- alloys Cu-Zn, Cu-Al, Cu-Sn. The content of Zn, Al, Sn - in at %

№	Cont. of Zn in alloy, at. %	E 10^{12} erg/cm^2	Cont. of Al in alloy, at. %	E 10^{12} erg/cm^2	Cont. of Sn in alloy, at. %	E 10^{12} erg/cm^2
1	O(Cu)	1.354	O(Cu)	1.354	O(Cu)	1.354
2	4.1	1.128	4.80	1.138	2.70	1.155
3	9.1	1.089	5.62 [9]	1.145 [9]	2.99 [9]	1.165 [9]
4	10.00 [9]	1.172 [9]	6.80	1.093	6.50	1.139
5	17.1	1.055	9.10 [9]	1.034 [9]	6.35 [9]	1.075 [9]
6	20.00 [9]	0.986 [9]	11.25	0.996	8.9	1.126
7	22.7	1.031	15.35	0.850	11.0	1.053

In conclusion we note, that using of Θ_p as a measure of rigidity of ($f \sim M\Theta_p^2$) link in accordance with physical argumentation, presented by us in [1], may appear to be convenient in application sense.

Evaluation dependencies C_{ij} and numerical values of the elastic module E for a range of solid solutions of Cu-Zn, Cu-Al and Cu-Sn systems obtained by the authors may be widely used at studying of physical properties of solid solutions, the analysis of their mechanical properties and other characteristics taking into account unharmonicity.

CONCLUSIONS

1. The possibility of application of f. c. c. lattice model with central interaction for evaluation of Cu-Zn, Cu-Al and Cu-Sn solid solutions elastic modulii using X-ray diffractometry data was showed/

2. Obtained concentration dependencies of solid solution elastic modules for Cu-Zn, Cu-Al, Cu-Sn systems may be widely used in the process of physical and mechanical properties of the given systems.

3. It is showed, that the substitution of Cu atoms with atoms of Zn, Al, Sn, their valence being more than the valence of Cu, leads to decreasing of elastic modules.

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Babiuk Todor – Cand. Sc. (Eng.), Assist. Professor, Department of physics.

Avdeev Sergiy – Assist. Professor, Department of physics.
Vinnytsia National Technical University.