Anisotropy of Propagation of Elastic Waves in Crystals with Chalcopyrite Structure

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Abstract – Anisotropy of propagation of elastic waves in chalcopyrite is investigated by method of the numerical solution of Christoffel's equation with use of experimental values of elastic constants at various temperatures. Special directions in this crystal are determined. There are five longitudinal normals and three acoustic axes in irreducible part of Brillouin zone. Propagation directions of pure transverse waves and characteristics of the internal conic refraction are also determined.

Copper iron disulphide (chalcopyrite, $CuFeS_2$) is a very interesting material from the physical point of view. Chalcopyrite crystallizes in a tetragonal lattice with space group $I\bar{4}2d$ (D_{2d}^{12}) and 2 formula units per unit cell. A full system of elastic stiffness constants has been determined from the analysis of X-ray Bragg reflection intensities at different temperatures in paper [1]. The given article by means of the numerical solution of Christoffel's equation deals with anisotropy of propagation of acoustic waves in $CuFeS_2$ with the use of elastic constants taken from [1] and presented in table 1 at two extreme temperatures 10 and 300 K.

Table 1. Elastic constants of chalcopyrite c_{ij}, 10^{11} dyn/sm^2 [1]

T, K	c_{11}	c_{12}	c_{13}	c_{33}	c_{44}	c_{66}
10	21.35	10.13	3.11	43.38	5.88	12.25
300	20.50	9.61	2.98	41.41	5.65	11.62

Christoffel's equation was written in spherical coordinate system and it was solved for the irreducible part of Brillouin zone. It is set by the change of spherical coordinates within $0° \le \varphi \le 45°$, $0° \le \theta \le 90°$. Some special directions have been also investigated. They are longitudinal normals, acoustic axes and propagation directions of pure transverse waves [2].

Christoffel's equation may be transformed to the scalar equation which determines a cone of longitudinal normals [2]. It has been established from the analysis of this equation that $CuFeS_2$ has 13 longitudinal normals. There are 5 longitudinal normals in the irreducible part of Brillouin zone. Their directions are given in Table 2.

The revision of realization conditions of acoustic axes showed the crystal $CuFeS_2$ has 9 acoustic axes, in the irreducible part of Brillouin zone there are 3 acoustic axes (Table 3).

Table 2. Directions of longitudinal normals in the irreducible part of Brillouin zone

10 K	1	2	3	4	5
θ°	0	90	90	64.51	55.85
φ°	0	0	45	0	45
300 K					
θ°	0	90	90	64.41	55.94
φ°	0	0	45	0	45

Table 3. Directions of acoustic axes in the irreducible part of Brillouin zone

Angel, °	Temperature, K					
	10			300		
θ	0	64.8	90	0	65.0	90
φ	0	0	38.1	0	0	38.8

The internal conic refraction takes place for the acoustic axes which are not longitudinal normals. That is, if the wave normal coincides with the crystal acoustic axe, the whole direction cone of the energy flow vector corresponds to it. Each direction responds to the definite vector of the quasi-transverse wave displacement.

The calculated refraction characteristics are shown in Table 4.

The polarization vector directions of the quasi-longitudinal wave are presented in the third column of this table, the phase velocities of transverse waves are given in the fourth column. The seventh one shows the rotation direction of the energy flow vector related to the wave normal depending on the angulations (the eighth column) of the polarization vector of the quasi-transverse wave. The last column gives corresponding values of group velocities.

The propagation conditions of pure transverse waves in tetragonal system crystals are carried out for four planes (100), (010), (110), $(1\bar{1}0)$ passing through the fourth order axe. They are also performed for the coordinate plane (001). Besides, pure transverse waves may spread along the directions on the surface of the fourth order cone. Its equation is presented in [2]. Numerical solution of this equation gives a pair of angles θ, φ indicating the propagation directions of pure transverse waves (Fig. 1).

The cross sections of the refraction surfaces (the surface of reverse phase velocity) are built according to the calculated values of the phase velocity in different directions. The cross sections of these surfaces with planes (100), (010), (001) are shown in Figs. 2 and 3 for temperatures 10 and 300 K, respectively.

Table 4. Characteristics of the internal conic refraction

T, K	Acoustic axe, θ°/φ°	$\bar{\mathbf{U}}_{QL}$, θ°/φ°	V^F_{QT}, 10^3 m/s	Refraction cone cross-section	Cone axe, θ°/φ°	Rotation sign	α, °	V^F_{QT}, 10^3 m/s
10	64.8/0	65.13/0	5.15	ellipse	52.04/0	left screw	0 45 90 135	5.28 5.48 6.54 5.48
	90/38.1	90/42.15	3.75	ellipse	90/27.77	right screw	0 45 90 135	3.75 3.82 4.01 3.82
300	65.0/0	65.66/0	5.03	ellipse	51.97/0	left screw	0 45 90 135	5.15 5.34 6.40 5.34
	90/38.8	90/42.37	3.68	ellipse	90/29.63	right screw	0 45 90 135	3.68 3.73 3.88 3.73

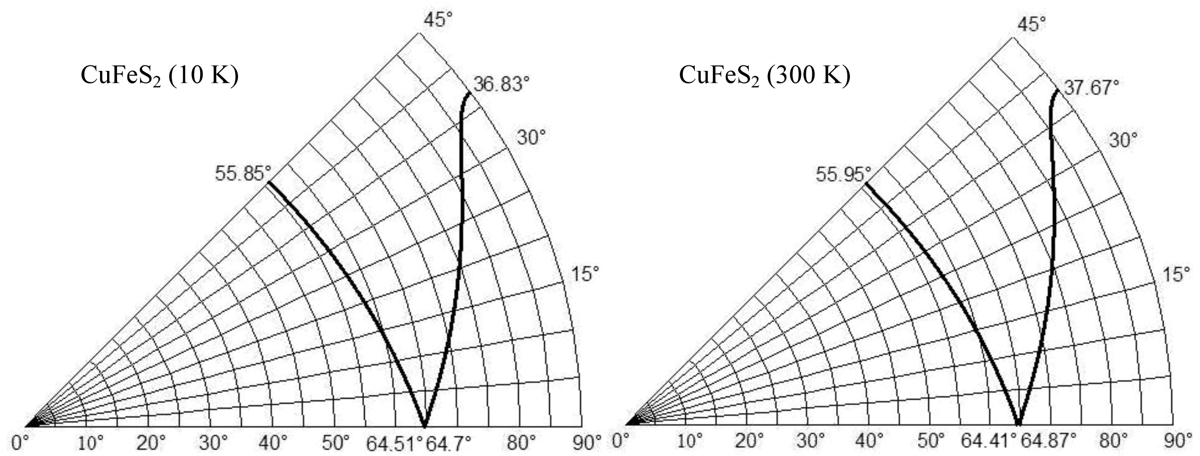

Fig. 1. Propagation directions of pure transverse waves

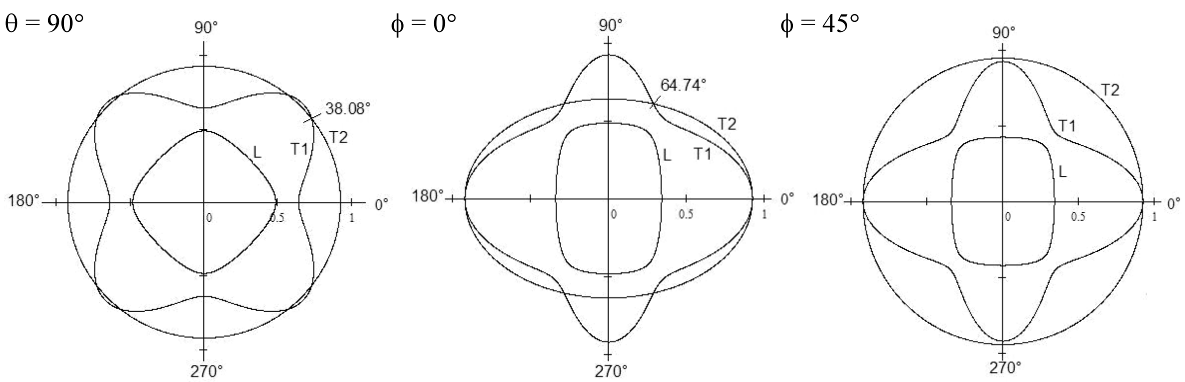

Fig. 2. The refraction surface cross sections by the symmetry surfaces in $CuFeS_2$ at 10 K

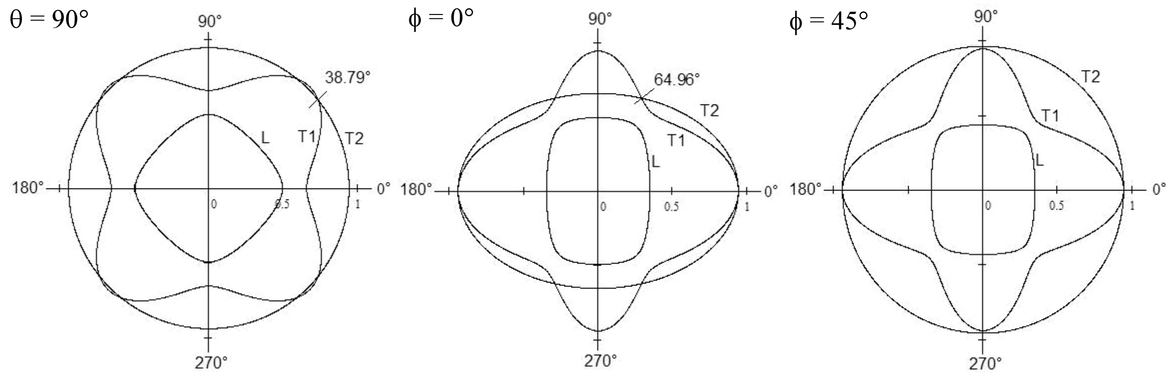

Fig. 3. The refraction surface cross sections by the symmetry surfaces in $CuFeS_2$ at 300 K

As it is seen from Figs. 2 and 3, the largest difference of the surfaces from the isotropic case takes place for the quasi-transverse (T_1, T_2) acoustic waves. The refraction surface for the quasi-longitudinal (L) waves presents slightly deformed ellipsoid.

From the results of the given paper, there are no qualitative changes in the propagation of acoustic waves in chalcopyrite in the wide range of temperatures from 10 to 300 K. The calculation results obtained are necessary for the construction of the intensity surfaces and for the analysis of phonon focusing. Besides, the given calculations may be used while studying different physical processes which occur with the participation of acoustic phonons, in particular, while calculating the time relaxation tensor while scattering on acoustic phonons.

References

[1] N.N. Sirota and Zh.K. Zhalgasbekova, Dokl. Akad. Nauk SSSR **321**, 513 (1991).

[2] F.I. Fedorov, *The theory of elastic waves in crystals*, Moscow, Nauka, 1965, 388 pp.