ELASTIC ANISOTROPY OF THE CUBIC, HEXAGONAL AND TETRAGONAL CRYSTALS[1]

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The paper deals with the experimental method of the investigation of the elastic anisotropy of crystals with cubic, hexagonal and tetragonal structure symmetry. The elastic invariant quantity proportional to the sum of the squared velocities of the three modes of acoustic waves in an arbitrary propagation direction fulfilling the condition of the invariance is used in order to follow the changes of the anisotropy parameters of a set of samples derived from some common basic material by means of different ingredients. The method significantly reduces the claims on the number and the orientation accuracy of the samples.

I. INTRODUCTION

Recently, we have investigated a great number of mixed crystals of alkaline earths fluorides with rare earths ingredients typical by their cubic symmetry [1], [2] and [3]. We have developed an experimental method which significantly reduces claims on the sample preparation. It is based on some relations between 2nd order elastic coefficients and acoustic waves velocities, significant because of the existence of elastic invariant quantities. In the present paper we can extend the method to other crystallographic structures characteristic by the existence of high order symmetry axes.

II. SECOND ORDER ELASTIC INVARIANTS

The elastic properties of the crystalline samples are described by means of a 2nd order elastic coefficients tensor. The elastic coefficients are connected with the acoustic waves velocities by means of the Christoffel equation [4]. The analysis of the relations leads to revealing some invariant quantities. It was proved in [5] that the quantity

$$\varrho\left(\sum_{i,j} V_{ij}^2\right) = c_{11} + c_{22} + c_{33} + 2(c_{44} + c_{55} + c_{66}) \qquad (1)$$

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is invariant to an arbitrary orientation of three ($i = 1, 2, 3$) orthogonal propagation directions of the acoustic waves of all three ($j = 1, 2, 3$) polarizations. Here ϱ is mass density, V_{ij} are acoustic waves velocities and c_{ij} are 2nd order elastic coefficients.

In addition it has been proved for the crystals with cubic symmetry [6] that the quantity

$$I_c = \varrho(v_L^2 + v_{T1}^2 + v_{T2}^2) = c_{11} + 2c_{44} \qquad (2)$$

is invariant to an arbitrary propagation direction orientation. Here v_L, v_{T1}, v_{T2} are the velocities of the longitudinal nad two transversal acoustic waves propagating in the same direction.

In the case of other crystallographic structures with significant symmetry axes such as the hexagonal, tetragonal and trigonal ones the quantity

$$I_T = \varrho(v_L^2 + v_{T1}^2 + v_{T2}^2) = c_{11} + c_{44} + c_{66} \qquad (3)$$

is invariant to an arbitrary propagation direction orientation in the plane normal to the significant symmetry axis. The hexagonal structure is characteristic by the 2nd order elastic coefficients relation $c_{12} = c_{11} - 2c_{66}$ which allows to express (3) in the form

$$I_{Th} = \frac{1}{2}(3c_{11} - c_{12} + 2c_{44}). \qquad (4)$$

From the experimental point of view it is important that the invariant quantities I_c, I_T can be determined by means of the three acoustic waves velocities measurement in only chosen propagation direction without an exact crystallographic sample orientation. From another point of view the invariant quantity (1) should be chosed in order to check the experimental results and those (2), (3) in order to check the supposed crystallographic structure or its deviation from the original structure symmetry caused by means of various disturbances.

III. ELASTIC ANISOTROPY OF CRYSTALS

The experimental methods of the crystal elastic properties investigation consist in the acoustic waves velocities and attenuations measurement. In the case of weakly disturbed crystals the relative variations of acoustic waves velocities are usually very low. On the other hand the weak crystal modifications cause their considerable anisotropy changes. It allows to develop a sensitive method of the testing anisotropy is connected with the difference of velocity of the acoustic waves of different polarizations and propagation directions.

In the case of cubic crystals the significant acoustic waves velocities are [4]

$$V_{L[100]} = \sqrt{\frac{c_{11}}{\varrho}} \qquad V_{T1[100]} = V_{T2[100]} = \sqrt{\frac{c_{44}}{\varrho}}$$

$$V_{L[110]} = \sqrt{\frac{1}{2\varrho}(c_{11} + c_{12} + 2c_{44})} \qquad V_{T1[110]} = \sqrt{\frac{1}{2\varrho}(c_{11} - c_{12})}$$

$$V_{T2[110]} = \sqrt{\frac{c_{44}}{\varrho}}$$

where V_{T2} represent the transversal polarization in the [001] direction and V_{T1} transversal polarization in the (001) plane. The cubic crystal anisotropy is described by means of the relative parameters

$$p = \frac{V^2_{T2[110]}}{V^2_{T1[110]}} = \frac{2c_{44}}{c_{11} - c_{12}} \qquad \xi = \frac{V^2_{L[100]}}{V^2_{T[100]}} = \frac{c_{11}}{c_{44}} \tag{5}$$

These parameters together with the invariant quantity (2) allow to express the 2nd order elastic coefficients

$$c_{11} = \frac{\xi}{\xi + 2} I_c \qquad c_{12} = \frac{p\xi - 2}{p(\xi + 2)} I_c \qquad c_{44} = \frac{1}{\xi + 2} I_c .$$

We can see that it is necessary to measure the acoustic waves velocities in both the [100] and the [110] directions to determine the anisotropy parameters (5).

We have shown for a set of samples based on CaF_2 or BaF_2 with cubic symmetry [2] only c_{11} coefficifent changes because of the rare earths ingredients concentration variations, whereas both c_{12} and c_{44} remain quasi constant. Under this assumption the relative anisotropy parameter changes can be expressed as

$$\frac{\xi}{\xi_0} = 1 + \frac{1}{\xi_0}(\xi_0 + 2)\frac{I_c - I_{c_0}}{I_{c_0}}$$

$$\frac{p}{p_0} = \left[1 + \frac{p_0}{2}(\xi_0 + 2)\frac{I_c - I_{c_0}}{I_{c_0}}\right]^{-1} \tag{6}$$

where I_{c_0}, ξ_0, p_0 are the values valid for the crystal without any ingredience. We can see it is sufficient to measure only the I_c variation in an arbitrary direction in order to follow the anisotropy parameter changes.

Hexagonal crystals are characteristic by the existence of the 6th symmetry axis. The acoustic waves velocities in directions normal to this axis are

$$V_L = \sqrt{\frac{c_{11}}{\varrho}} \qquad V_{T1} = \sqrt{\frac{1}{2\varrho}(c_{11} - c_{12})} \qquad V_{T2} = \sqrt{\frac{c_{44}}{\varrho}} .$$

The anisotropy parameters have the form

$$p = \frac{V^2_{T2}}{V^2_{T1}} = \frac{2c_{44}}{c_{11} - c_{12}} \qquad \xi = \frac{V^2_L}{V^2_{T2}} = \frac{c_{11}}{c_{44}} . \tag{7}$$

With respect to invariant quantity (4) the elastic coefficients can be expressed

$$c_{11} = \frac{\xi}{\xi + 1 + 1/p} I_{Th} \qquad c_{12} = \frac{1}{p}\frac{p\xi - 2}{\xi + 1 + 1/p} I_{Th}$$

$$c_{44} = \frac{1}{\xi + 1 + 1/p} I_{Th} .$$

In the case of the investigation of the influence of weak structure disturbances on the elastic anisotropy we can suppose a dominant dependency of one of the elastic coefficients.

If we suppose both c_{12} and c_{44} to be quasi constant, the anisotropy parameters of the modified crystal are

$$\frac{\xi}{\xi_0} = 1 + \frac{2}{3\xi_0}\left(\xi_0 + 1 + \frac{1}{p_0}\right)\frac{I_{Th} - I_{Th_0}}{I_{Th_0}}$$

$$\frac{p}{p_0} = \left[1 + \frac{p_0}{3}\left(\xi_0 + 1 + \frac{1}{p_0}\right)\frac{I_{Th} - I_{Th_0}}{I_{Th_0}}\right]^{-1} \tag{8}$$

where the zero subscript indicates the values valid for the not disturbed fundamental crystal.

Tetragonal crystals are characteristic by the existence of the 4th symmetry axis. The acoustic waves velocities in directions normal to the symmetry axis are

$$V_{L[100]} = \sqrt{\frac{c_{11}}{\varrho}} \qquad V_{T1[100]} = \sqrt{\frac{c_{66}}{\varrho}} \qquad V_{T2[100]} = \sqrt{\frac{c_{44}}{\varrho}} .$$

$$V_{L[110]} = \sqrt{\frac{1}{2\varrho}(c_{11} + c_{12} + 2c_{66})} \qquad V_{T1[110]} = \sqrt{\frac{1}{2\varrho}(c_{11} - c_{12})}$$

$$V_{T2[110]} = \sqrt{\frac{c_{44}}{\varrho}}$$

The anisotropy parameters have the form

$$p = \frac{V^2_{T2[110]}}{V^2_{T1[110]}} = \frac{2c_{44}}{c_{11} - c_{12}} \qquad \xi = \frac{V^2_{L[100]}}{V^2_{T2[100]}} = \frac{c_{11}}{c_{44}}$$

$$p' = \frac{V^2_{T1[100]}}{V^2_{T1[110]}} = \frac{2c_{66}}{c_{11} - c_{12}} \qquad \xi' = \frac{V^2_{L[100]}}{V^2_{T1[100]}} = \frac{c_{11}}{c_{66}} \tag{9}$$

$$p'' = \frac{V^2_{T2[100]}}{V^2_{T1[100]}} = \frac{c_{44}}{c_{66}}$$

We can express the 2nd order elastic coefficients with respect to the invariant quantity (3) by means of the relations

$$c_{11} = \frac{\xi}{\xi + 1 + \xi/\xi'} I_T \qquad c_{12} = \frac{1}{p}\frac{p\xi - 2}{\xi + 1 + \xi/\xi'} I_T$$

$$c_{44} = \frac{1}{\xi + 1 + \xi/\xi'} I_T \qquad c_{66} = \frac{\xi}{\xi'}\frac{1}{\xi + 1 + \xi/\xi'} I_T$$

Similarly we can follow the anisotropy parameters variations by means of the invariant changes measurement. If we suppose the dominant c_{11} variation to be caused by the weak structure disturbances and quasi constant values of the other elastic coefficients, the anisotropy parameters can be expressed as

$$\frac{p}{p_0} = \frac{p'}{p'_0} = \left[1 + \frac{p_0}{2}(\xi_0 + 1 + \xi_0/\xi'_0)\frac{I_T - I_{T_0}}{I_{T_0}}\right]^{-1} \tag{10}$$

$$\frac{\xi}{\xi_0} = \frac{\xi'}{\xi'_0} = 1 + \frac{1}{\xi_0}(\xi_0 + 1 + \xi_0/\xi'_0)\frac{I_T - I_{T_0}}{I_{T_0}}$$

IV. CONCLUSION

The elastic properties investigation gives us information on the crystallographic structure of solids. In the case of a set of very similar samples derived from the common basic material by means of different ingredients the elastic anisotropy parameters sensitively indicate the structure changes. The most serious difficulty of their investigation is connected with the necessity of an exact crystallographic sample orientation. We have utilized the elastic invariant quantitaties to develop the presented method, which significantly reduces the claims on the measured samples. The anisotropy parameters variations are followed by means of the three modes of acoustic waves velocities measurement in only one propagation direction corresponding to the invariance condition.

The method has been experimentally proved in the investigation of the set of alkali fluorides with rare earths ingredients. We have extended the range of its utilization to the cases of the crystallic materials with tetragonal and hexagonal symmetries.

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УПРУГАЯ АНИЗОТРОПИЯ КУБИЧЕСКИХ, ГЕКСАГОНАЛЬНЫХ И ТЕТРАГОНАЛЬНЫХ КРИСТАЛЛОВ

Работа посвящена экспериментальному методу исследования упругой анизотропии в кристаллах с кубической, гексагональной и тетрагональной симметрией. Введена величина, независимая от упругости, пропорциональная сумме квадратов скоростей трех мод акустических волн в произвольном направлении распространения, удовлетворяющая условию периодичности. Эта величина используется для исследования изменения параметров анизотропии набора образцов, полученных у одного основного материала при использовании различных примесей. Метод сощуственно упрощает требования на число и точность ориентации образцов.