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USING INDICATORY SURFACES FOR THE STADY OF ANISOTROPY OF THERMAL CRYSTAL EXPANSION

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For the graphic image of thermal expansion anisotropy the three-dimensional revolving models of indicatory surfaces were constructed. The form and orientation of these surfaces depends on the crystal symmetry in accordance with the principle of Neumann.
Keywords: indicatory surfaces, thermal expansion, anisotropy.
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INTRODUCTION

Materials generally change their size when subjected to a temperature change while the pressure is held constant. Common engineering solids usually have coefficients of thermal expansion that do not vary significantly over the range of temperatures where they are designed to be used, so where extremely high accuracy is not required, practical calculations can be based on a constant, average, value of the coefficient of expansion.

Thermal expansion of crystals is described by nine coefficients, which form a symmetric tensor of the second order. For the evident graphic image of anisotropy of thermal expansion, it is convenient to use indicatory surfaces. Radius-vector of this surface is proportional to the size of the relative lengthening of crystal in this direction at heating.

1. METHODS OF INVESTIGATION

To a first approximation, the change in length measurements of an object ("linear dimension" as opposed to, e.g., volumetric dimension) due to thermal expansion is related to temperature change by a "linear expansion coefficient". It is the fractional change in length per degree of temperature change. Assuming negligible effect of pressure, we may write:

$$\alpha_n = \frac{\Delta l / l}{\Delta T} . \tag{1}$$

Where l is a particular length measurement and $\Delta l / l$ is the rate of change of that linear dimension per unit change in temperature.

For a definite choice of the coordinate system (the choice is determined by installation rules and associated to the elements of the symmetry of the crystal) amount of independent coefficients α_n decreases [1], Table 1.

Coefficient of thermal expansion in any direction, [2]:

$$\alpha_n=\sum\alpha_{ij}\cdot n_i\cdot n_j\ . \qquad (2)$$

Where α_{ij} are coefficients of thermal expansion of crystals, formative the second-order tensor; n_i, n_j are components of the vector of unit length determining in some direction in the crystal.

Table 1

The equations of indicatory surfaces of thermal expansion

Category	View of the tensor of thermal expansion	The number of independent parameters	The equations indicatory surfaces
Higher	$\begin{pmatrix}\alpha_{xx} & 0 & 0\\ 0 & \alpha_{xx} & 0\\ 0 & 0 & \alpha_{xx}\end{pmatrix}$	1	$\alpha_n=\alpha_{xx}$
Middle	$\begin{pmatrix}\alpha_{xx} & 0 & 0\\ 0 & \alpha_{xx} & 0\\ 0 & 0 & \alpha_{zz}\end{pmatrix}$	2	$\alpha_n=\alpha_{xx}\cdot(n_x^2+n_y^2)+\alpha_{zz}\cdot n_3^2$
Lowest	$\begin{pmatrix}\alpha_{xx} & 0 & 0\\ 0 & \alpha_{yy} & 0\\ 0 & 0 & \alpha_{zz}\end{pmatrix}$	3	$\alpha_n=\alpha_{xx}\cdot n_x^2+\alpha_{yy}\cdot n_y^2+\alpha_{zz}\cdot n_z^2$
	$\begin{pmatrix}\alpha_{xx} & 0 & \alpha_{xz}\\ 0 & \alpha_{yy} & 0\\ \alpha_{zx} & 0 & \alpha_{zz}\end{pmatrix}$	4	$\alpha_n=\alpha_{xx}\cdot n_x^2+\alpha_{yy}\cdot n_y^2+\alpha_{zz}\cdot n_z^2+2\cdot\alpha_{xz}\cdot n_x\cdot n_z$
	$\begin{pmatrix}\alpha_{xx} & \alpha_{xy} & \alpha_{xz}\\ \alpha_{yx} & \alpha_{yy} & \alpha_{yz}\\ \alpha_{zx} & \alpha_{zy} & \alpha_{zz}\end{pmatrix}$	6	$\alpha_n=\alpha_{xx}\cdot n_x^2+\alpha_{yy}\cdot n_y^2+\alpha_{zz}\cdot n_z^2+2\cdot\alpha_{xy}\cdot n_x\cdot n_y+2\cdot\alpha_{xz}\cdot n_x\cdot n_z+2\cdot\alpha_{yz}\cdot n_y\cdot n_z$

For the construction of three-dimensional revolving models of indicatory surfaces would be convenient to use application package MathCad. Great mathematical capabilities of this package make it a convenient tool for physical research [3, 4].

Within this package the program was created, that allows to construct of indicatory surfaces of thermal expansion. Analysis of the received indicatory surfaces allows defining the symmetry and the anisotropy of the properties, and, if necessary, establishing the directions of its extreme value.

2. RESULTS AND DISCUSSION

Thermal expansion of crystals of the highest category symmetry (cubic crystal system) is described by a single coefficient. α. For any other cubic crystal, indicatory surface has a form of a sphere. Thus, the crystals of higher category evenly broaden on all directions, saving the primary form.

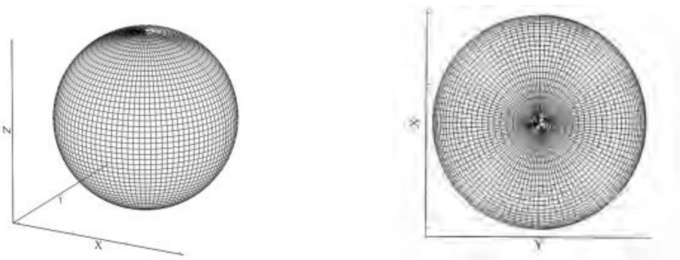

Fig. 1. The indicatory surface of thermal expansion of the cubic crystal and its projection on the plane (XOY).

For the crystals of middle category (crystals of this category have an third, fourth or sixth order axis of rotation, the axis Z is directed along its) let us consider number of interesting cases:

a) All the coefficients of thermal expansion more than zero, at that $\alpha_{xx} < \alpha_{zz}$. For example, for a crystal of zinc: α_{xx}= $14 \cdot 10^{-6}$, °C^{-1}, α_{zz}= $55 \cdot 10^{-6}$ °C^{-1} , [5], Fig. 2.

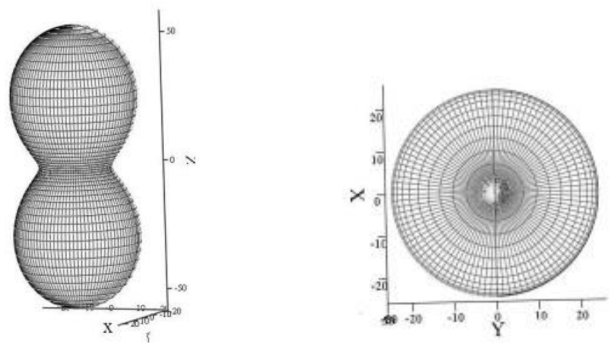

Fig. 2. The indicatory surface of thermal expansion of zink and its projection on the plane (XOY).

For a crystal of zinc indicatory surface is elongated along the axis Z. This axis coincides with the axis of the sixfold. With a uniform heating of zinc in this direction crystal pull stronger than in the perpendicular direction.

b) All the coefficients of thermal expansion more than zero, and $\alpha_{zz} < \alpha_{xx}$. As, for example, for a crystal α-quartz: α_{xx}=14·10^{-6} °C^{-1}, α_{zz}= 9·10^{-6} °C^{-1}.

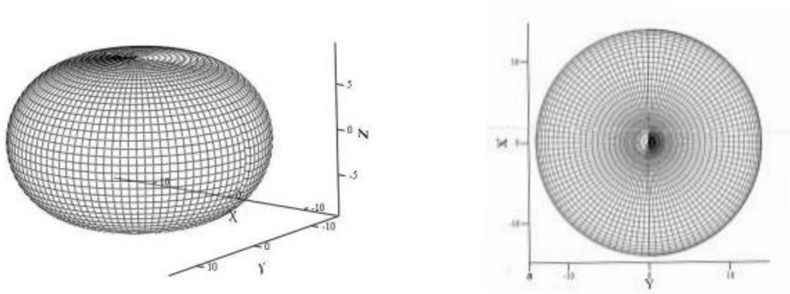

Fig. 3. The indicatory surface of thermal expansion of α-quartz and its projection on the plane (XOY).

It is seen, that surface of thermal expansion in this case is the ellipsoid flattened along the axis of Z. This direction of minimum increase of crystal of quartz at heating. And maximally – in perpendicular direction.

c) We will especially distinguish a case, when one of coefficients of thermal expansion less zero. As an example, the indicatory surface of thermal expansion of a crystal calcite $CaCO_3$, which is widely used in an optical instrument production. Its coefficients of thermal expansion: α_{xx}= -5,2·10^{-6} °C^{-1}, α_{zz}= 22,6·10^{-6} °C^{-1}. The indicatory surface of thermal expansion of a crystal calcite is multi-cavity surface with positive and negative areas of thermal expansion, Figure 4. It is seen, that along the axis of Z thermal expansion of calcite is maximal. Perpendicular to this axis is the region of negative thermal expansion (compression). Thus, at heating, calcite broadens in one direction, and in other – compressed. Also near the axis of Z there is a cone of directions with half-angle 75°56′, along which the expansion (compression) is zero. In these directions at heating, a crystal does not change.

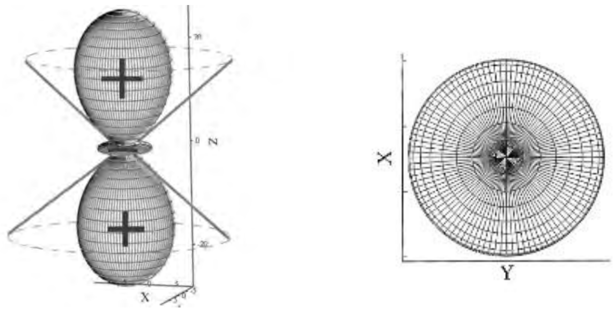

Fig. 4. The indicatory surface of thermal expansion of calcite and its projection on the plane (XOY).

Thus, indicatory surfaces of thermal expansion of crystals middle category are spheroids. The axis of rotation is the main axis of symmetry (Z).

For crystals of the lowest category, depending on the symmetry and, accordingly, the number of independent coefficients of thermal expansion, there are also a number of cases:

a) Three independent coefficients of thermal expansion, as, for example, for the orthorhombic crystal system.

For example, for a crystal of aragonite in this category α_{xx}= $35\cdot10^{-6}$ °C^{-1}, α_{yy}= $17\cdot10^{-6}$ °C^{-1}, α_{zz}=$10\cdot10^{-6}$ °C^{-1}, characterized by the presence of three mutually perpendicular twofold axes of symmetry. The indicatory surface of thermal expansion of aragonite is shown in Fig. 5.

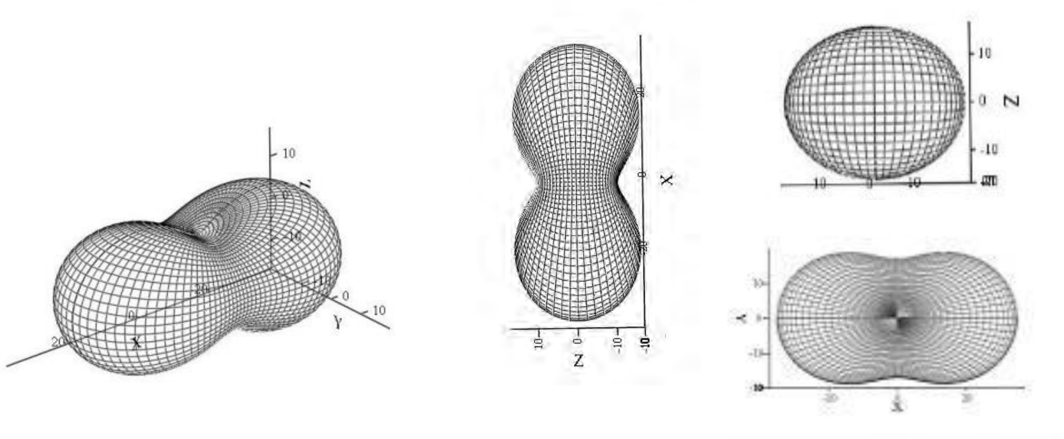

Fig. 5. The indicatory surface of thermal expansion of aragonite and its projection on the planes (XOY), (XOZ) и (ZOY).

It is seen that all the projections are ellipses. Indicatory surface of such crystals is a triaxial ellipsoid with axes coinciding with the coordinate axes, which coincide with the twofold axis of symmetry.

b) In less symmetrical crystals this category (the monoclinic crystal system) indicatory surface is described by four thermal coefficients. For example, for a crystal of potassium tartrate: α_{xx}= $12\cdot10^{-6}$ °C^{-1}, α_{yy}= $44{,}8\cdot10^{-6}$°C^{-1}, α_{zz}= $32\cdot10^{-6}$ °C^{-1}, α_{xz}= $-\ 12\cdot10^{-6}$ °C^{-1}. The indicatory surface of such crystals in projection has one ellipse only – perpendicular to the axis of Y, that coincides with the only axis of symmetry in these crystals, Fig. 6.

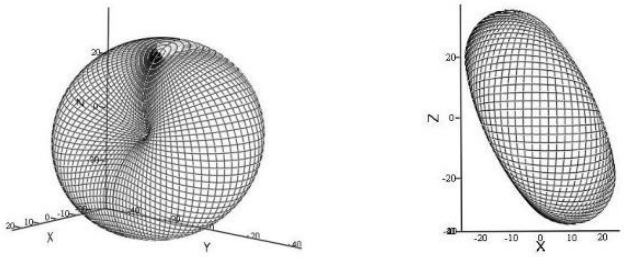

Fig. 6. The indicatory surface of thermal expansion of potassium tartrate and its projection on the plane (XOZ).

CONCLUSION

The anisotropy of thermal expansion of single crystals in some way connected with their symmetry, according to Neumann's principle:

1. Thermal expansion of crystals of the highest category is isotropic.
2. When heated, the crystals of middle and lower category can expand in all directions or in certain directions to shrink and expand in other ones.
3. An indicatory surface of thermal expansion of such crystals is spheroids if all α_{ij} – positive or surface with several (positive and negative) parts, if some α_{ij} – negative.
4. There are determined directions in a crystal in last case along which thermal expansion is equal to zero.

References

1. W. A. Wooster, *Tensors and group theory for the physical properties of crystals* (Claredon Press, Oxford, 1973).
2. Y. I. Sirotin, M. P. Shaskol'skaya, *Fundamentals of Crystal Physics* (Nauka, Moscow, 1979).
3. S. N. Polulyakh, *Application packages in physics* (Pyramid Crimea, Simferopol, 1998).
4. E. M. Maksimova, *Tensor properties of crystals. Method. Handbook for practical lessons on the course «Physics of crystals»* (Taurida National V. I. Vernadsy University, Simferopol, 2002).
5. N. V. Perelomova, M. M. Tagiyeva, *Book of problems in crystal physics* (Nauka, Moscow, 1982).

Максимова О. М. Використання вказівних поверхонь для дослідження анізотропії теплового розширення кристалів. / О. М. Максимова, А. І. Замковська // Вчені записки Таврійського національного університету імені В. І. Вернадського. Серія : Фізико-математичні науки. – 2014. – Т. 27 (66), № 2. – С. 92-98.

Показана можливість дослідження анізотропії теплового розширення кристалів за допомогою графічних поверхонь, радіус-вектори яких характеризують відносні величини властивості в заданому напрямку. За формою указательной поверхні можна виявити екстремальні напрямки, в яких величина, що визначає властивість, приймає максимальне або мінімальне значення. Симетрія указательной поверхні повинна містити в собі всі елементи симетрії кристала відповідно до принципу Неймана.

Ключові слова: вказівна поверхня, теплове розширення, анізотропія.

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Показана возможность исследования анизотропии теплового расширения кристаллов с помощью графических поверхностей, радиус-векторы которых характеризуют относительные величины свойства в заданном направлении. По форме указательной поверхности можно выявить экстремальные направления, в которых величина, определяющая свойство, принимает максимальное или минимальное значение. Симметрия указательной поверхности должна содержать в себе все элементы симметрии кристалла в соответствии с принципом Неймана.
Ключевые слова: указательная поверхность, тепловое расширение, анизотропия.

Список литературы

1. Wooster W. A. Tensors and group theory for the physical properties of crystals / W. A. Wooster. – Oxford : Claredon Press, 1973. – 354 p.
2. Сиротин Ю.И. Основы кристаллофизики / Ю. И. Сиротин, М. П. Шаскольская. – М.: Наука, 1979. – 640 с.
3. Полулях С. Н. Пакеты прикладных программ в физике / С. Н. Полулях. – Симферополь : Изд-во «Пирамида-Крым», 1998. – 104 с.
4. Максимова Е.М. Компьютерное моделирование тензорных свойств кристаллов / Е. М. Максимова. – Симферополь: ТНУ, 2002. – 23 с.
5. Переломова Н. В. Задачник по кристаллофизике / Н. В. Переломова, М. М. Тагиева. – М. : Наука, 1982. – 288 с.

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