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Conditions of elastic mechanical stability and elastic properties of crystal structures with different symmetry

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A critical analysis of the conditions of elastic stability of crystal structures of different symmetry as restrictions imposed on their elastic constants c_{ij} has been carried out. It is shown that the conditions of elastic stability of all crystals, except for cubic ones, are described by polynomials from the second to sixth powers of their elastic constants c_{ij}. Necessary and sufficient conditions for the elastic stability of crystals of different symmetry are presented explicitly.

Keywords: Elastic stability, Symmetry, Elastic constants, Stability conditions.

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1. Introduction

To study elastic properties of the crystal materials is a priority task in the solid-state physics. Along with experimental studies, the last two decades have witnessed distribution *ab initio* of calculations of elastic constants and modules of solid-phase compounds with a various structure by using the density functional theory.

The electron structure and elastic properties of simulated crystal compounds are calculated by a full-potential linearized augmented-plane-wave method including a local-orbital method (FP-LAPW + *lo*) [1,2], which are based on the density functional theory (DFT).

Recently, theoretical methods have been intensely developed to simulate possible structures of compounds and their mechanical properties depending on the composition and to find structures to be favorable in terms of energy. Quite reliable results can be obtained by means of an evolution prediction algorithm of crystal structures as implemented in the USPEX software [3–5].

The energy of the crystal compounds simulated by means of the evolution algorithm is calculated withing the density functional theory [6] using the PBE version [7] in the Generalized Gradient Approximation (GGA)) and the Projector-Augmented Wave method (PAW)) [8], as implemented in the VASP code (Vienna Ab initio Simulation Package) [9,10].

There are hundreds of original studies in the literature, which are devoted to evaluate the elastic properties of a variety of crystal substances.

The structure and elastic properties of osmium nitride OsN_2 with cubic and rhombic lattices, ultra-hard iridium nitrides IrN_2 and IrN_3 with cubic, hexagonal, tetragonal, monoclinic and several rhombic structures, platinum nitride PtN with structures of a zinc-blende type, rhombic and cubic structures were studied in the papers [11–13]. The structure and mechanical stability of the elastic properties of niobium nitrides NbN with the NaCl and CsCl cubic structures and the hexagonal δ- and ε-structures as well as of tetragonal and cubic modifications of boron nitride are discussed in the papers [14,15].

Tetragonal, orthorhombic and monoclinic phases of silver azide AgN_3 are discussed in terms of their elastic properties and mechanical stability in the paper [16], which shows significant difference in their stability and usability of the orthorhombic modification of the silver azide in the solid-state reaction of explosion decomposition. The elastic properties and mechanical stability of the cubic, orthorhombic and monoclinic chlorates and perchlorates $NaClO_3$, $KClO_3$, $LiClO_4$, $NaClO_4$, $KClO_4$ are studied in the paper [17].

The structure and mechanical properties of the orthorhombic and trigonal phases CaB_2H_2, the orthorhombic and monoclinic polymorphs Li_2FeSiO_4, which can be alternative cathode materials, are discussed in the papers of Vajeeston et al. [18,19]. The ab initio calculations of the mechanical properties of the organic & inorganic hybrid perovskites $CH_3NH_3BX_3$ ($B = \mathrm{Sn, Pb}$; $X = \mathrm{Br, I}$) with cubic, tetragonal and orthorhombic structures are carried out within the density functional theory in the paper [20]. The elastic properties and mechanical stability of the semiconductor cubic solid solutions $In_xAl_{1-x}As_ySb_{1-y}$ are studied in the paper [21], while the paper [22] discusses the mechanical stability of gypsum $CaSO_4 \cdot 2H_2O$.

Methods of calculation of the elastic stiffness and mechanical stability constants can be applied not only to the solid-phase crystal compounds, but to fullerites and materials based thereon [23–25].

Structures of numerous carbide phases M_nC_m ($M = \mathrm{Zr, Hf, Nb, Ta}$) [26–32] were predicted and calculated

by means of theoretical methods of analysis of the electron and crystal structure.

The persistence of the crystal structure is importantly characterized by an elastic (mechanical) stability, whose criteria are defined by the elastic constants. The conditions of the mechanical stability (persistence) of the crystal structures are usually worded as requirements to the elastic stability of the crystal lattices and depend on their symmetry [33]. Criteria of the Born elastic stability are well known for cubic crystals, and the monograph [33] explicitly provides the stability criteria of cubic, hexagonal, tetragonal and trigonal crystals. However, for crystals with lower symmetry (especially, rhombic and monoclinic ones), the conditions of the mechanical persistence are defined inexactly and even erroneously (see, for example, the paper [12]). Derivation of necessary and sufficient conditions of the elastic stability of the crystals is a nontrivial and quite difficult task. That is why many authors just cite wrong stability conditions from the paper [12] and use them. In connection therewith, with no sophisticated mathematical derivation, the present paper provides necessary and sufficient conditions of the elastic stability of crystals of a various symmetry.

2. Results and discussion

Depending on the crystal symmetry, there are 7 qualitatively different matrices of the elastic constants, which differ in a number of independent non-zero variables c_{ij} and correspond to the seven crystal systems [33]. The paper [34] discusses 9 qualitatively different matrices (two matrices each, with a different number of non-zero variables c_{ij} for tetragonal and trigonal crystals with a different point symmetry). However, Fedorov showed in the monograph [33] that for correct selection of orientation of the coordinate system for all the seven point crystal symmetry groups of the tetragonal system there is one matrix of the elastic constants; for the trigonal crystals with five point symmetry groups there is also one matrix of the elastic constants.

The elastic behavior of the lattice is described by the matrix of the elastic constants of the second order:

$$c_{ij} = \frac{1}{V_0}\left(\frac{\partial_2 E}{\partial\varepsilon_i \partial\varepsilon_j}\right), \tag{1}$$

where E and V_0 — energy of the elastic deformation of the crystal and its equilibrium volume, ε — deformation. In the general case, the matrix ($\mathbf{C}$) of the elastic stiffness constants has a size of 6×6, is a symmetrical one and can include 21 independent elastic constants c_{ij}.

The energy of elastic deformation referred to a crystal volume unit, for arbitrary infinitely small deformation is determined in [33,35,36] as

$$E/V \sim \frac{1}{2}\sum_{i,j=1}^{6} c_{ij}\varepsilon_i\varepsilon_j. \tag{2}$$

The matrix ($\mathbf{C}$) of the elastic stiffness constants of low-symmetry crystals of a triclinic system includes the biggest number of the independent non-zero elastic constants — 21 (c_{11}, c_{12}, c_{13}, c_{14}, c_{15}, c_{16}, c_{22}, c_{23}, c_{24}, c_{25}, c_{26}, c_{33}, c_{34}, c_{35}, c_{36}, c_{44}, c_{45}, c_{46}, c_{55}, c_{56} and c_{66}) and takes the following form:

$$(\mathbf{C})_{\text{tricl}} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & c_{15} & c_{16} \\ c_{12} & c_{22} & c_{23} & c_{24} & c_{25} & c_{26} \\ c_{13} & c_{23} & c_{33} & c_{34} & c_{35} & c_{36} \\ c_{14} & c_{24} & c_{34} & c_{44} & c_{45} & c_{46} \\ c_{15} & c_{25} & c_{35} & c_{54} & c_{55} & c_{56} \\ c_{16} & c_{26} & c_{36} & c_{46} & c_{56} & c_{66} \end{pmatrix}. \tag{3}$$

The matrix ($\mathbf{S}$) of elastic compliance constants is correlated to the matrix ($\mathbf{C}$) in a simple relationship $(\mathbf{S})^{-1} = (\mathbf{C})$ or $(\mathbf{C})(\mathbf{S}) = 1$. Taking this into account, the matrix ($\mathbf{S}$) of the elastic compliance constants has the same size of 6×6 and includes 21 independent elastic constants s_{ij}. For crystals with the symmetry higher than the triclinic one, a part of the constants c_{ij} or s_{ij} goes to 0.

As per the studies [35–37], the crystal is stable if and only if the energy of the elastic deformation is positive, i.e. above zero for all the actual values ε_I and ε_j, if only all ε_I and ε_j are nonzero. It imposes additional limitations on the constants c_{ij} and s_{ij}.

The mechanical stability of the crystal of an arbitrary symmetry has a necessary condition for it, which is not a sufficient one: all diagonal elements of the matrix of the elastic stiffness constants are to be positive, i.e.

$$c_{ii} > 0 \quad (i = 1{-}6). \tag{4}$$

The sufficient conditions of the mechanical stability are fulfilled if all the own values of the matrix ($\mathbf{C}$) of the elastic stiffness constants are positive. In order to determine own values of a square matrix C, a characteristic matrix $C-\lambda E$ is used, where E — a unit matrix, λ — some unknown variable [38,39]. A polynom $|C-\lambda E|$ is a characteristic polynom of the matrix C, and its roots are characteristic roots, i.e. are own values of the matrix C.

The elastic matrix of the cubic crystals includes only 3 independent elastic constants c_{11}, c_{12} and c_{44}:

$$(\mathbf{C})_{\text{cub}} = \begin{pmatrix} c_{11} & c_{12} & c_{12} & & & \\ c_{12} & c_{11} & c_{12} & & & \\ c_{12} & c_{12} & c_{11} & & & \\ & & & c_{44} & & \\ & & & & c_{44} & \\ & & & & & c_{44} \end{pmatrix}. \tag{5}$$

For the cubic crystals, the constants c_{11}, c_{12} and c_{44} are positive. The mechanical stability conditions of the cubic crystals determined in the papers [40,41] are known as the

Born stability criteria:

$$c_{11} > c_{12}, \quad c_{44} > 0, \quad c_{11} + 2c_{12} > 0. \tag{6}$$

The cubic system is the only one, for which the mechanical stability conditions are linear.

The elastic matrix of the hexagonal crystals includes the 5 independent elastic constants c_{11}, c_{12}, c_{13}, c_{33}, c_{44}:

$$(\mathbf{C})_{\text{hex}} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & & & \\ c_{12} & c_{11} & c_{13} & & & \\ c_{13} & c_{13} & c_{33} & & & \\ & & & c_{44} & & \\ & & & & c_{44} & \\ & & & & & (c_{11}-c_{12})/2 \end{pmatrix}. \tag{7}$$

The necessary and sufficient conditions of the elastic stability of the hexagonal crystals take the following form:

$$c_{11} > |c_{12}|, \quad c_{44} > 0, \quad (c_{11} + c_{12})c_{33} > 2c_{13}^2. \tag{8}$$

The necessary and sufficient conditions of the elastic stability of the low-symmetry (tetragonal, trigonal (rhombohedral), orthorhombic and monoclinic) crystals have been earlier discussed in the papers [12,34].

The matrix of the elastic stiffness constants of the tetragonal crystals depends on the 6 independent constants c_{11}, c_{12}, c_{13}, c_{33}, c_{44} and c_{66}:

$$(\mathbf{C})_{\text{tetr}} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & & & \\ c_{12} & c_{11} & c_{13} & & & \\ c_{13} & c_{13} & c_{33} & & & \\ & & & c_{44} & & \\ & & & & c_{44} & \\ & & & & & c_{66} \end{pmatrix}. \tag{9}$$

The mechanical stability conditions of the tetragonal crystals take the following form:

$$c_{11} > |c_{12}|, \ c_{44} > 0, \ c_{66} > 0, \ (c_{11} + c_{12})c_{33} > 2c_{13}^2. \tag{10}$$

The mechanical stability criteria (10) of the tetragonal crystals contain the quadratic polynoms from c_{ij}, but in the papers [12,13,15] the mechanical stability conditions of the tetragonal phases are represented in an erroneous linear form as

$$c_{ii} > 0, \ (c_{11} - c_{12}) > 0, \ (c_{11} + c_{33} - 2c_{13}) > 0, \\ (2c_{11} + 2c_{12} + c_{33} + 4c_{13}) > 0. \tag{11}$$

The trigonal (rhombohedral) crystals have 6 independent elastic constants c_{11}, c_{12}, c_{13}, c_{14}, c_{33}, c_{44}:

$$(\mathbf{C})_{\text{trig}} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & c_{14} & & \\ c_{12} & c_{11} & c_{13} & -c_{14} & & \\ c_{13} & c_{13} & c_{33} & & & \\ c_{14} & -c_{14} & & c_{44} & & \\ & & & & c_{44} & c_{14} \\ & & & & c_{14} & (c_{11}-c_{12})/2 \end{pmatrix}. \tag{12}$$

Their mechanical stability conditions take the following form:

$$c_{11} > |c_{12}|, \ c_{44} > 0, \ (c_{11} + c_{12})c_{33} > 2c_{13}^2, \\ (c_{11} - c_{12})c_{44} > 2c_{14}^2. \tag{13}$$

The elastic stiffness matrix of the orthorhombic crystals includes 9 independent constants c_{11}, c_{12}, c_{13}, c_{22}, c_{23}, c_{33}, c_{44}, c_{55} and c_{66}:

$$(\mathbf{C})_{\text{orthorh}} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & & & \\ c_{12} & c_{22} & c_{23} & & & \\ c_{13} & c_{23} & c_{33} & & & \\ & & & c_{44} & & \\ & & & & c_{55} & \\ & & & & & c_{66} \end{pmatrix}. \tag{14}$$

The paper [34] has shown that taking into account the condition $c_{ii} > 0$ $(i = 1{-}6)$ (4), the necessary and sufficient conditions of the mechanical stability of the rhombic crystals include quadratic and cubic polynoms and take the following form:

$$\left.\begin{array}{l} c_{11} > 0, \ c_{44} > 0, \ c_{55} > 0, \ c_{66} > 0, c_{11}c_{22} > c_{12}^2, \\ c_{11}c_{12}c_{33} + 2c_{12}c_{13}c_{23} - c_{11}c_{23}^2 - c_{22}c_{13}^2 - c_{33}c_{12}^2 > 0 \end{array}\right\}. \tag{15}$$

The nonlinear conditions (15) are fundamentally different from the linear conditions:

$$c_{ii} > 0, \ c_{ii} + c_{jj} - 2c_{ij} > 0, \\ c_{11} + c_{22} + c_{33} + 2(c_{12} + c_{13} + c_{23}) > 0, \tag{16}$$

proposed by the authors of the paper [11] and repeated in the paper [12]. Note that the stability conditions of the rhombic crystals used in the papers [11,12], are, in the best case scenario, only necessary, but not sufficient. The erroneous linear conditions (16) seem to have been obtained as a result of incorrect generalization of the cubic criteria (6) to other orthogonal (tetragonal and rhombic) crystals. Evaluation of the mechanical stability of the rhombic crystals by means of the linear conditions (16) can lead to erroneous conclusions.

In particular, the erroneous linear conditions (16) have been used to evaluate the mechanical stability

of such orthorhombic phases as platinum nitride PtN (sp.gr. $Fddd$) [13], silver azide AgN_3 (sp.gr. $Ibam$) [16], perchlorates of alkali metals (sp.gr. $Pnma$, $Cmcm$) [17], calcium borohydride CaB_2H_2 (sp.gr. $Cmc2_1$) [18], complex-replaced lithium silicate Li_2FeSiO_4 (sp.gr. $Pmn2_1$, $Pna2_1$, $Pnma$) [19], zirconium carbide Zr_3C_2 (sp.gr. $Fddd$) [29].

The wrong conditions of the mechanical stability for the crystals with the symmetry below the cubic one are often given in papers of various authors. The wrong linear conditions (11) of the mechanical stability of the tetragonal system's crystals are given in the paper [12], but for the tetragonal crystals the stability conditions (10) include the quadratic polynoms from c_{ij}. The same erroneous linear polynoms are used to write the mechanical stability conditions for the tetragonal (sp.gr. $P4_2/mmc$) platinum nitride PtN [13] and for the tetragonal (sp.gr. $I\bar{4}2d$) crystals of boron nitride BN [15]. The wrong stability criteria are given in the paper [14] for the hexagonal niobium nitride. The paper [42] does not take into account the limitations $c_{11} > |c_{12}|$ for the mechanical stability conditions of the trigonal crystals.

The crystals of the monoclinic systems are described by elastic matrices having 13 independent elastic constants c_{11}, c_{12}, c_{13}, c_{15}, c_{22}, c_{23}, c_{25}, c_{33}, c_{35}, c_{44}, c_{46}, c_{55} and c_{66}:

$$(\mathbf{C})_{\text{mon}} = \begin{pmatrix} c_{11} & c_{12} & c_{13} & & c_{15} & \\ c_{12} & c_{22} & c_{23} & & c_{25} & \\ c_{13} & c_{23} & c_{33} & & c_{35} & \\ & & & c_{44} & & c_{46} \\ c_{15} & c_{25} & c_{35} & & c_{55} & \\ & & & c_{46} & & c_{66} \end{pmatrix}. \quad (17)$$

The monoclinic phases are mechanically stable, if their elastic constants c_{ii} meet the following inequalities, which include together with the linear polynoms, polynoms of the second, third and fourth degrees

$$c_{ii} > 0 (i = 1{-}6), \; c_{22} + c_{33} > 2c_{23},$$
$$c_{11} + c_{22} + c_{33} > 2(c_{12} + c_{13} + c_{23}), \quad (18a)$$
$$c_{33}c_{55} > c_{35}^2, \quad c_{44}c_{66} > c_{46}^2,$$
$$c_{22}c_{33}c_{55} + 2c_{23}c_{25}c_{35} > c_{22}c_{35}^2 + c_{55}c_{23}^2 + c_{33}c_{25}^2, \quad (18b)$$
$$2\big[c_{15}c_{25}(c_{33}c_{12} - c_{13}c_{23}) + c_{15}c_{35}(c_{22}c_{13} - c_{12}c_{23}) + c_{25}c_{35}(c_{11}c_{23} - c_{12}c_{13})\big] > c_{15}^2(c_{22}c_{33} - c_{23}^2) + c_{25}^2(c_{11}c_{33} - c_{13}^2) + c_{35}^2(c_{11}c_{22} - c_{12}^2) + pc_{55}, \quad (18c)$$

where $p = c_{11}c_{22}c_{33} - c_{11}c_{23}^2 - c_{22}c_{13}^2 - c_{33}c_{12}^2 + 2c_{12}c_{13}c_{23}$.

The mechanical stability conditions of the crystals of the cubic and hexagonal systems are determined in the Born papers [40,41], and the Fedorov monograph [33] additionally obtains the mechanical stability conditions of the tetragonal and trigonal crystals. The stability conditions of the high- and low-symmetry crystals are also described in the paper [12], but wrong conditions are given for the tetragonal and orthorhombic crystals. The authors [34] have discussed an excess number of the matrices of the elastic constants for the tetragonal and trigonal crystals and have not provided the stability criteria of the monoclinic crystals. In the present study we have analyzed the known mechanical stability conditions, marking and excluding the erroneous conditions, for some crystal systems we have calculated correct stability conditions and for the first time we have collected the mechanical stability criteria of the crystal systems from the cubic to monoclinic one.

3. Conclusion

Thus, we have described the elastic stability conditions of the crystals with the various symmetry as limitations imposed on their elastic constants c_{ij}. These conditions are described by the linear polynoms of the elastic constants for the cubic crystals and combinations of the linear and quadratic polynoms for the hexagonal, tetragonal and trigonal (rhombohedral) crystals. The elastic stability conditions of the orthorhombic crystals include linear, quadratic and cubic polynoms. The mechanical stability criteria of the monoclinic and triclinic crystals additionally include the polynoms of the fourth and sixth order, respectively.

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Conflict of interest

The authors declare that they have no conflict of interest.

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