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Comparison of features arising in phonon spectra of crystals belonging to the argyrodite family for various combinations of orbits filled with Ag (Cu) atoms

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Abstract. The paper is devoted to model phonon spectra calculations of argyrodite family crystals, namely: Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I). The specificity of the crystalline structure of these crystals is realization of variable partial populating different crystallographic orbits with Cu, I and Ag atoms (in 24 (g) and 48 (h) Positions Multiplicity, Wyckoff letter, Site symmetry of the space group $F\bar{4}3m$), which are associated with high superionic conductivity in crystals of this family. Compared in this paper are model phonon spectra calculated with account of three different configurations of orbital populations with Cu and Ag atoms (6 + 1, 5 + 2 and 4 + 3), by choosing the same lattice model for the unit cell and the set of force constants of each crystal. The calculations were performed by finding the eigenvalues of the generalized dynamic matrix perturbed by the modulation function of the mass defect obtained in the concept over spatial symmetry. It is shown that the phonon spectra do not undergo significant qualitative changes, which can serve as indirect evidence of the possibility to realize the jumping mechanism of super-ionic conductivity in these crystals in the high-temperature phase.

Keywords: super-spatial symmetry, phonon spectrum, force constant, modulation vector, dynamic matrix.

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1. Introduction

Simplification of mathematical description, formulation of certain rules of selection, reference points and exact relationships in theory, including the theory of condensed matter, is associated with the theory of symmetry and its generalizations [1]. In recent years, equally productive has been the idea of lattice models [2, 3], which also allows for a number of simplifications and precise solutions. We show the possibility to obtain some simplifications in the method of calculating the model dispersion dependences for phonons in complex crystals, in the concept of spatial symmetry [4–9] by using the idea of lattice models [2, 3].

The crystallographic description of the structure of complex crystals in a certain space group is associated with the choice of the type of unit cell and the set of Wyckoff positions; the latter determine the crystallographic orbits and thus the number of atoms in the unit cell and their coordinates [10].

To describe the structure of the unit cell, we use a combination of the idea of spatial symmetry and the lattice model. To define a lattice model of n^3 order (for cubic syngony) in the metric of a convenient protocrystal, which will provide the minimum possible value of n, we describe the minimum lattice model in the concept of spatial symmetry [4–9].

In recent years, researchers have continued to pay attention to complex multi-component compounds of interest for practical use, including the low-temperature superconductors, superionic crystal structures, and disordered and low-dimensional systems. Note that all of them are characterized by the presence of specific defects in the crystal structure, namely, a set of partially filled crystallographic orbits. The appearance of partial filling of the crystallographic orbits positions formally leads to a significant decrease in the spatial symmetry and the emergence of additional perturbation in the lattice associated with this defect. This feature of the structure, as a rule, in further studies is neglected by performing

them in the classical description. Interestingly, this type of structural defect is also described in the literature as imperfect crystals.

2. Material and methods

Partial filling of the crystallographic orbits positions with certain atoms is clearly manifested in the argyrodites family [10]. Compounds of this family are characterized by a feature that metal atoms partially occupy the positions of crystallographic orbits of different power (symmetry) without filling them completely. This in turn, leads to or promotes super-ionic conductivity in these compounds [11].

To describe the unit cell of the argyrodite family, we have chosen a lattice model of 8×8×8 order, of 512 dimension, where it is convenient to choose the following basis of the face-centered lattice (*a*, *a*, 0); (*a*, 0, *a*); (0, *a*, *a*). Thus, to describe the unit cell, we obtain a face-centered lattice model that is similar to [6] of (8*a*, 8*a*, 0); (8*a*, 0, 8*a*); (0, 8*a*, 8*a*) dimension of 512 order. The points of possible localization are the metrics of the basic face-centered structure protocrystal) (*a*, *a*, 0); (*a*, 0, *a*); (0, *a*, *a*).

The localization of atoms of the argyrodite family (Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I) type) is shown by the selected points and given in Tables 1 and 2 in the work [6].

To describe the composition of atoms in the unit cell of crystals (Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I) type), we choose the FCC superlattice (8*a*, 8*a*, 0; 8*a*, 0, 8*a*; 0, 8*a*, 8*a*) in the metric of the protocrystal (*a*, *a*, 0; *a*, 0, *a*; 0, *a*, *a*) described as (3 + 3) structure with (3 + 3) dimensional direct and inverse bases:

$$a_1=\left(a,a,0,\ \frac{\bar{b}}{8},\frac{\bar{b}}{8,0}\right),\cdots\cdots\ a_1^*=\left(\frac{\bar{\pi}}{a},\frac{\pi}{a},\frac{\pi}{a},0,0,0\right);$$

$$a_2=\left(a,0,a,\frac{\bar{b}}{8,0},\frac{\bar{b}}{8}\right),\qquad a_2^*=\left(\frac{\pi}{a},\frac{\bar{\pi}}{a},\frac{\pi}{a},0,0,0\right);$$

$$a_3=\left(0,a,a,0,\frac{\bar{b}}{8},\frac{\bar{b}}{8}\right),\qquad a_3^*=\left(\frac{\pi}{a},\frac{\pi}{a},\frac{\bar{\pi}}{a},0,0,0\right);$$

$$a_4=(0,0,0,b,b,0),\qquad a_4^*=\left(\frac{\bar{\pi}}{8a},\frac{\pi}{8a},\frac{\pi}{8a},\frac{\bar{\pi}}{b},\frac{\pi}{b},\frac{\pi}{b}\right);$$

$$a_5=(0,0,0,b,0,b),\qquad a_5^*=\left(\frac{\pi}{8a},\frac{\bar{\pi}}{8a},\frac{\pi}{8a},\frac{\pi}{b},\frac{\bar{\pi}}{b},\frac{\pi}{b}\right);$$

$$a_6=(0,0,0,0,b,b),\qquad a_6^*=\left(\frac{\pi}{8a},\frac{\pi}{8a},\frac{\bar{\pi}}{8a},\frac{\pi}{b},\frac{\pi}{b},\frac{\bar{\pi}}{b}\right),$$

which determine the 512-fold multiplication of volumes.

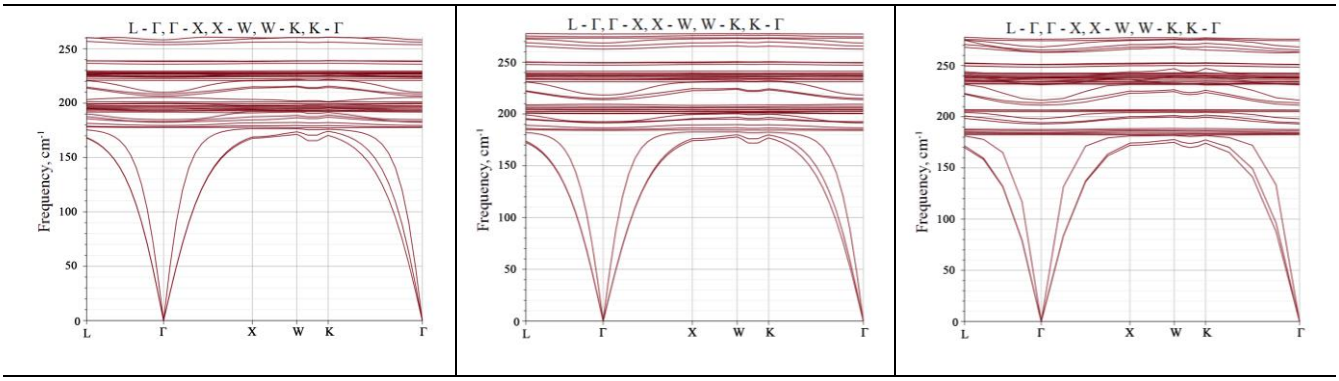
The set of 512 possible positions of atoms covers 30 orbits, and the set of 512 modulation vectors is separated into 30 stars similar to Table 2 in [6].

Consideration of the structure and calculations for the super-spatial model were carried out by solving the secular equation, similarly to [6–9, 12], of the order 1536×1536 with the involvement of 512 potential positions, 14 of which are occupied by the atoms of structures Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I), namely: I [0, 0, 0], $Cu_2(Ag_2)$ [142] (3, 3, 0), $Cu_2(Ag_2)$ [153] (0, –3, –3), $Cu_2(Ag_2)$ [146],, $Cu_1(Ag_1)$ [370] (4, 4, 0), $Cu_1(Ag_1)$ [371] (4, 0, 4), $Cu_1(Ag_11)$ [372] (0, 4, 4)$^{+,++}$, $Cu_1(Ag_11)$ [373] (–4, 4, 0), $Cu_1(Ag_11)$ [374] (–4, 0, 4), $Cu_1(Ag_11)$ [375] (0, –4, 4)$^{++}$, $Se_2(S_2)$ [490] (6, 2, 2), $Se_2(S_2)$ [491] (2, 6, 2), $Se_2(S_2)$ [492] (2, 2, 6), $Se_2(S_2)$ [493] (–6, 2, 2), Ge(Si) [498] (4, 4, 4), Si(Ge)[512] (8, 0, 0) (similar to Fig. 1 in the work [6]). (Here and in Tables 1 and 2 [6], the occupied positions are marked with asterisks, and empty in various schemes of calculations are marked with crosses.)

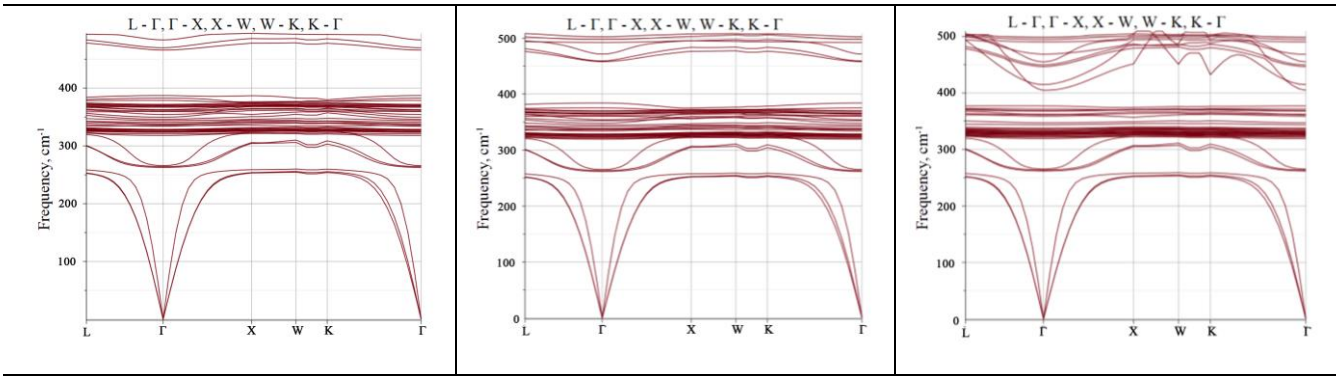
Dynamic matrices of the protocrystal were calculated at 512 points of the Brillouin zone. Modifying the population of crystallographic positions with atoms (in schemes (6 + 1), (5 + 2) and (4 + 3) that cover the average population range of $Cu_1(Ag_1)$ and $Cu_2(Ag_2)$ orbits), which is displayed in the form of a mass defect matrix and correcting the values of the force constants in the equidistant approximation, phonon spectra were obtained for the highly symmetric directions of the FCC lattice Brillouin zone (Fig. 1).

The values of force constants α_n are given in the order of ascending distances between the position of orbits 1(0, 0, 0) and n + 1 with account of all the possible variants of the distances between the pairs of occupying atoms. The force constants were chosen in the equidistant approximation; the interaction was determined only by the distance and did not depend on the type of interacting pairs of atoms. For example, for the compound Ag_7GeSe_5I, α_6 is the force constant describing this interaction at the distance $2a\sqrt{3}$ and equal to 3.1 N/m, so the others are, correspondingly, Ag_7GeSe_5I Cu_7SiS_5I force constants: [52.1, 0, 0, 0, 0, 3.1, 2.2, 1.7, 1, 1, 0, 0, 0, 0, .7, 0, 1, 5, 0, 0, 0, 2, 0, 0, 10, 33.0, 6, 23.50] n/m. As a result of model analysis for the structures of Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I), taking into account the occupancy of the orbit of the $Cu_2(Ag_2)$ atom in the metric of the protocrystal with the FCC basis (*a*, *a*, 0), (*a*, 0, *a*), (0, *a*, *a*) and the superlattice with the FCC basis (8*a*, 8*a*, 0), (8*a*, 0, 8*a*), (0, 8*a*, 8*a*), the rearrangement of the phonon spectrum inherent to Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I) crystals was observed, which was caused by the change in the corresponding mass characteristics of Cu and Ag atoms and by a certain expected correlation between the force constants. The results of calculations performed in this work are in a satisfactory agreement with the experimental data obtained for the frequency range of ~150…350 cm^{-1} at the Γ point [3]. The wide frequency ranges of values obtained in this work can indicate the effective possibility of their changes by changing the occupancy of the Cu(Ag) atoms (*i.e.*, by "jumps" of atoms between the considered orbits),

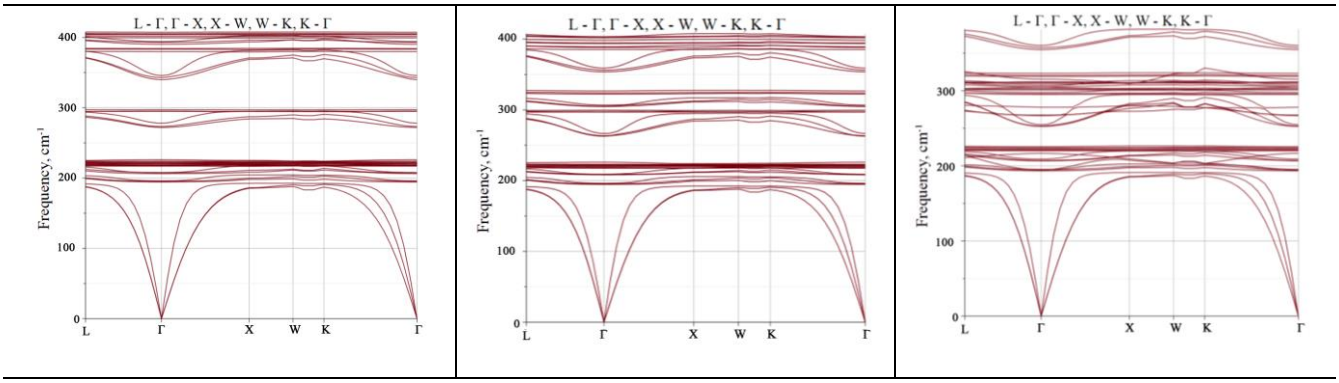
Ag_7GeSe_5I Power Constants: [25.1,0,0,0,0,0.10,4,0.10,0.6,1,0,0,0,0,0.7,0,3,7,0,0,0,2,0.23,0,0.8,3,0,5.5]n/m



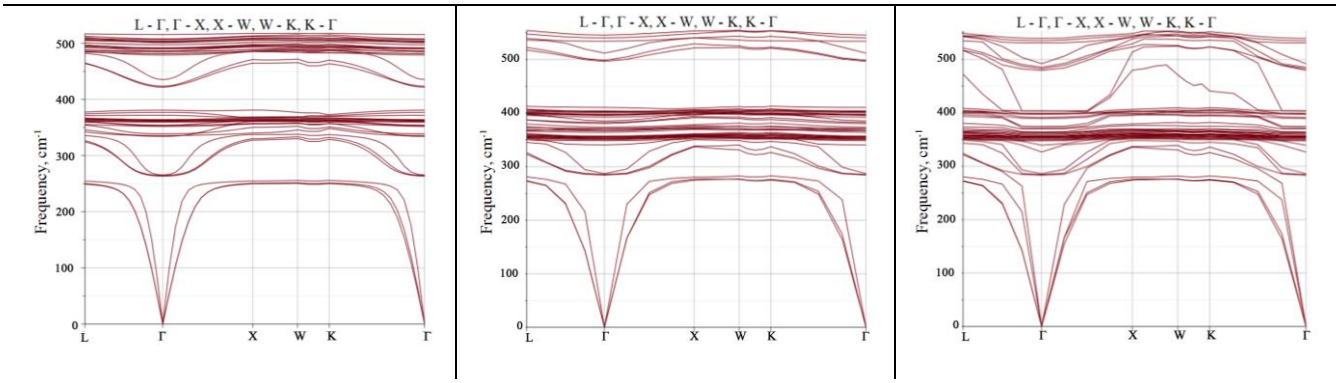
Cu_7GeSe_5I Power Constants: [70.1,0,0,0,0,3.1,2.2,1.7,0.6,1,0,0,0,0,0.7,0,1,5,0,0,0,2,0.23,0,8,30.8,0.6,22]n/m



Ag_7SiS_5I Power Constants: [19.1,0,0,0,0,0.1,5.5,0.1,6.5,0.1,0,0,0,0,1,0,1,3.5,0,0, 0, 4,0.23,0,0 .8,3.2,1,5.2]n/m



Cu_7SiS_5I Power Constants: [52.1,0,0,0,0,3.1,2.2,1.7,1,1,0,0,0,0,0.7,0,1,5,0,0,0,2,0,0,10,33.0,0.6,23.50]n/m



(6 + 1)	(5 + 2)	(4 + 3)
masses [1]: = 127(I);	masses [1]: = 127(I);	masses [1]: = 127(I);
masses [512]: = 72.6(Ge(Si));	masses [512]: = 72.6(Ge(Si));	masses [512]: = 72.6(Ge(Si));
masses [498]: = 79(Se(S));	masses [498]: = 79(Se(S));	masses [498]: = 79(Se(S));
masses [490]: = 79(Se(S));	masses [490]: = 79(Se(S));	masses [490]: = 79(Se(S));
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masses [493]: = 79(Se(S));	masses [493]: = 79(Se(S));	masses [493]: = 79(Se(S));
masses [370]: = 63.5(Cu(Ag));	masses [370]: = 63.5(Cu(Ag));	masses [370]: = 63.5(Cu(Ag));
masses [371]: = 63.5(Cu(Ag));	masses [371]: = 63.5(Cu(Ag));	masses [371]: = 63.5(Cu(Ag));
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masses [374]: = 63.5(Cu(Ag));	masses [375]: = 63.5(Cu(Ag));	masses [142]: = 63.5(Cu(Ag));
masses [375]: = 63.5(Cu(Ag));	masses [142]: = 63.5(Cu(Ag));	masses [153]: = 63.5(Cu(Ag));
masses [142]: = 63.5(Cu(Ag))	masses[153] : = 63.5(Cu(Ag)).	masses [146]: = 63.5(Cu(Ag)).

Fig. 1. Model phonon dispersion dependences of Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I) crystals, calculated for highly symmetric directions of the Brillouin zone, the list of populated positions and the list of force constant values.

which is accompanied by the high ionic conductivity in the super-ionic Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I).

3. Conclusions

As a result of the model analysis of the structures of Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I) with account of various schemes for occupancy of the Cu(Ag) atom orbit in the metric of the protocrystal with the FCC basis (*a*, *a*, 0), (*a*, 0, *a*), (0, *a*, *a*) – protocrystal in superlattice with the FCC real structure (8*a*, 8*a*, 0), (8*a*, 0, 8*a*), (0, 8*a*, 8*a*), an attempt to calculate the phonon spectra of cubic syngony crystals with the possibility of going beyond the classical description of the crystal structure has been shown. Thus, the rearrangement of the phonon spectrum of Cu_7GeSe_5I and Ag_7GeSe_5I crystals, which is caused by the values of the corresponding mass characteristics of Cu and Ag atoms and a certain correlation of the force constants, has been obtained. It is worth to note that satisfactory coincidence of the range of calculated frequencies with the experimental range of frequencies (150 to 350 cm^{-1}) at the Γ point has been observed [3]. The obtained dispersion curves are characterized by significant proximity for all three studied calculation schemes, for both types of crystals (energy width of the range of changes in optical frequencies, the existence of three wide absorption bands), which may reflect the possibility of effective population rearrangement by Cu (Ag), which in turn can contribute to high ionic conductivity in the super-ionic phase of crystals Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I) (by "jumping" of atoms between the considered orbits). At the same time, the increase in deviation from the classical disintegration of atoms in the crystals of cubic syngony indicates an increase in the magnitude of the splitting between the phonon branches and a complication of the dispersion dependences of the latter (most obviously for the Cu_7GeSe_5I structure). In general, we can say that the change in the partial population of different orbits does not lead to a significant change in the overall energy characteristics of the phonon subsystem, and therefore can stimulate the mobility of Cu (Ag) atoms, noting that the preference in this analysis can be given to the system Ag_7GeSe_5I (Ag_7SiS_5I) as compared to the Cu_7GeSe_5I (Cu_7SiS_5I) one.

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Katanytsia A.F.: Calculation method software.
Shkyrta I.M.: Carrying out calculations.
Pal Yu.O.: Carrying out calculations.
Studenyak I.P. : Reconciliation of experimental data and results of calculations.
Timko M., Kopčanský P.: Material support for the possibility of calculations.

Порівняння особливостей фононних спектрів кристалів сімейства аргіродитів при різних комбінаціях орбіт, заселених атомами Ag (Cu)

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Анотація. Роботу присвячено модельним розрахункам фононних спектрів кристалів сімейства аргіродитів, а саме Ag_7GeSe_5I and Cu_7GeSe_5I (Ag_7SiS_5I and Cu_7SiS_5I). Специфікою кристалічної структури цих кристалів є реалізація змінної часткової заселеності різних кристалографічних орбіт атомами Cu, I та Ag (у 24(g) і 48(h) Positions Multiplicity, Wyckoff letter, Site symmetry просторової групи $F\bar{4}3m$), з якими пов'язується висока суперіонна провідність у кристалах цього сімейства. У роботі наведено співставлення модельних фононних спектрів, розрахованих з урахуванням трьох різних конфігурацій заселеності орбіт атомами Cu та Ag (6 + 1, 5 + 2 і 4 + 3), при виборі однакової решіткової моделі для елементарної комірки та набору силових постійних кожного з кристалів. Розрахунки здійснювалися шляхом знаходження власних значень узагальненої динамічної матриці, збуреної модуляційними функціями дефекту мас, які отримано в концепції надпросторової симетрії. Показано, що фононні спектри не зазнають значних якісних змін, що може служити непрямим доказом можливості реалізації стрибкового механізму суперіонної провідності в цих кристалах у високотемпературній фазі.

Ключові слова: надпросторова симетрія, фононний спектр, силова постійна, вектор модуляції, динамічна матриця.

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