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# Modification of Phonon Spectra of Ag7GeSe5I and Cu7GeSe5I Crystals with Different Partial Population of Crystallographic Orbits

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***Abstract-*** In the concept of superspatial symmetry the crystal structure of $Ag_7GeSe_5I$ та $Cu_7GeSe_5I$ superionic conductors has been analyzed. To calculate the phonon spectra, the model of FCC superlattice ($8a$, $8a$, 0; $8a$, 0, $8a$; 0, $8a$, $8a$) in the metric of protocrystal ($a$, $a$, 0; $a$, 0, $a$; 0, $a$, $a$) has been developed. For the developed model, the general (3+3)-dimensional basis, the array of modulation vectors and mass modulation functions have been presented. The model calculations of phonon spectra dispersion for $Ag_7GeSe_5I$ та $Cu_7GeSe_5I$ crystals in schemes with various partial occupation of crystallographic orbits by Cu(Ag) atoms have been performed. The dispersion dependences of phonon spectra for $Ag_7GeSe_5I$ та $Cu_7GeSe_5I$ crystals in the high-symmetric directions of Brillouin zone have been presented. The genesis of phonon branches of vibrational spectra has been analyzed.

***Keywords-*** *Argyrodites, Crystal Structure, Superlattice, Superspatial Symmetry, Phonon Spectrum, Maple*

## I. INTRODUCTION

Crystal structures of the argyrodite family are distinguished by the fact that they realize the partial population of certain positions of the crystallographic orbits of the cubic syngony. Particular attention in this regard is drawn to the implementation of high-temperature superionic phase, which leads to high mobility of conduction ions. The latter is of great interest to these structures by experimenters and theorists.

The main task of the theoretical study of this work is the lattice of these superionic crystals, taking into account the change in the partial populations of different positions of their crystal structure.

## II. METHOD OF CALCULATION OF COMPLEX CRYSTALS PHONON SPECTRA IN THE CONCEPT OF SUPERSPATIAL SYMMETRY

Compositional peculiarities of complex crystals and systems of solid solutions by the mechanism of filling with different sorts atoms and vacancies of translationally equivalent positions given by the basis of the protocrystal are covered by the concept of superspatial symmetry [1-3]. Different combinations of protocrystal bases and real crystalline formation together with all possible variants of compositional filling of crystallographic positions can be taken into account and thus supplement the classical crystallographic description, which does not take into account this fact. Using the complete set of modulation vectors allows to determine the amplitudes of mass modulation functions and on their basis to generate the generalized dynamic matrix of real physical object as well as mass perturb-bation matrix: the first one is given as a superposition of the dynamic matrix of the protocrystal, defined at different points of the Brillouin zone (ZB) related by modulation vectors, while the second one is described by amplitudes of mass modulation functions [4,5].

In the concept of superspatial symmetry, the dispersion curves of the phonon spectrum of crystalline formation are defined as solutions of the matrix equation under the condition of equality to zero of the determinants belonging to the following type:

$$\left|D_{\alpha\beta}(k+q_i) - \omega^2\delta_{\alpha\beta}\delta_{ij} - \omega^2\rho_{(i-j)}\delta_{\alpha\beta}\right| = 0, \quad (1)$$

where $D_{\alpha\beta}(k+q_i)$ are dynamic matrices of the monoatomic protocrystal determined at the points of ZB $(k+q_i)$, $\rho_{(i-j)} = \rho_i\left(q_i, \Delta^* b^*_{ij}\right)$ are the amplitudes of the mass modulation function specified for the modulation vector $(q_i - q_j)$, $k$ is the wave vector, $q_j$ are the modulation vectors, α, β – coordinates $x, y, z$. The solution of the matrix equation relatively to $\omega^2(k)$ allows to determine the dispersion dependences of the phonon spectrum, and taking into account the various variants of compositional filling – to monitor their genesis [5].

Dynamic matrices of the protocrystal $D_{\alpha\beta}(k+q_i)$ are determined from the equation:

$$D_{\alpha\beta}(k+q_i) = \sum_{(n\neq 0)} \alpha_n \frac{n_\alpha n_\beta}{n^2}\left(1 - e^{i(k+q_i)n}\right), \quad (2)$$

where $\alpha_n$ is the power constant of the atom interaction in 0 position and $n$ – adjacent atom, $n_\alpha$, $n_\beta$ are the projections of the vector $n$ on the axis α, β.

In equidistant approximation to the model, the power characteristic depends only on the distance between atoms, and then interaction of different sort atoms in equidistant positions is the same. This enables to form a dynamic matrix in a quasi-diagonal form. In a non-equidistant approximation, $\alpha_n$ is defined by both the distance between positions and the difference between the physical characteristics of the objects occupying them.

The values of amplitudes of mass characteristics $\rho(q_j)$ are obtained by solving the system of equations with respect to the amplitudes of mass modulation functions $\rho(q_j) = \rho_j$:

$$m(r_k) = \sum_{j=1}^{s} \rho(q)\ e^{iq_j r_k}, \qquad (3)$$

where s is the number of possible positions of atoms in the superlattice, $m(r_k)$ are mass characteristics in these positions, $q_j$ is an array of modulation vectors, the number of which coincides with the number of positions in the superlattice.Maintaining the Integrity of the Specifications

## III. Modified Model Phonon Spectra of Superionic Crystals of $Ag_7GeSe_5I$ and $Cu_7GeSe_5I$ Type

Let us describe some representatives of the family of argyrodite in the concept of superspatial symmetry, based on the model of natural FCC (8a,8a,0; 8a,0,8a; 0.8a.8a)-superlattice, when considering the power field in an equidistant approximation.

Representatives of the argyrodite family belong to the crystalline structures characterized by the partial occupancy of a part of crystallographic orbits by atoms of one sort. The crystalline structure of the argyrodite type $Cu_7GeSe_5I$ and $Ag_7GeSe_5I$ superionic conductors [6] consists of an anionic frame and filling of Ag (Cu) atoms in the positions of the cationic framework with population, which is characteristic for the crystals of the argyrodite family [5] (Table 1) (note that for the argyrodites family the average number of atoms in the orbits of Cu1 and Cu2 type is in the range of 4.3-4 , 8 (Cu1) to 2.7-2.2 (Cu2)), setting them in the positions of the lattice model [7] of 8x8x8 dimension (Fig. 1, Table 2).

The array of 512 possible positions of atoms covers 30 orbits, and the set of 512 modulation vectors is divided into 30 stars (Table 2).

When calculating the phonon spectra of $Ag_7GeSe_5I$ and $Cu_7GeSe_5I$ crystals for the crystal structure description, the model of FCC superlattice (8*a*, 8*a*, 0; 8*a*, 0, 8*a*; 0, 8*a*, 8*a*) in the protocrystal metric (*a*, *a*, 0; *a*, 0, *a*; 0, *a*, *a*) with (3+3)-dimensional straight and inverted basis was chosen:

$$a_1 = \left(a, a, 0, \bar{b}/8, \bar{b}/8, 0\right); \qquad a_1^* = \left(\bar{\pi}/a, \pi/a, \pi/a, 0, 0, 0\right);$$
$$a_2 = \left(a, 0, a, \bar{b}/8, 0, \bar{b}/8\right); \qquad a_2^* = \left(\pi/a, \bar{\pi}/a, \pi/a, 0, 0, 0\right);$$
$$a_3 = \left(0, a, a, 0, \bar{b}/8, \bar{b}/8\right); \qquad a_3^* = \left(\pi/a, \pi/a, \bar{\pi}/a, 0, 0, 0\right);$$
$$a_4 = \left(0, 0, 0, b, b, 0\right); \qquad a_4^* = \left(\bar{\pi}/8a, \pi/8a, \pi/8a, \bar{\pi}/b, \pi/b, \pi/b\right);$$
$$a_5 = \left(0, 0, 0, b, 0, b\right); \qquad a_5^* = \left(\pi/8a, \bar{\pi}/8a, \pi/8a, \pi/b, \bar{\pi}/b, \pi/b\right);$$
$$a_6 = \left(0, 0, 0, 0, b, b\right); \qquad a_6^* = \left(\pi/8a, \pi/8a, \bar{\pi}/8a, \pi/b, \pi/b, \bar{\pi}/b\right)$$

which determine 512-fold multiplication of volumes. The total of 512 possible positions of atoms covers 30 orbits, including both orbits of 10 (Cu1) and 18 (Cu2) type and the set of 512 modulation vectors is separated into 30 stars (Table 2).

Consideration of the structure and calculations for the superspatial model were carried out by solving the secular Eq. (1), similarly [8], 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 $Cu_7GeSe_5I$, namely: I [0, 0, 0], Cu2(Ag2)[142] (3, 3, 0), Cu2(Ag2)[153] (0, -3, -3)$^{*,**}$, Cu2(Ag2)[$^{**}$Cu1(Ag1)[370] (4,4,0), Cu1(Ag1)[371] (4,0,4), Cu1(Ag1)[372] (0,4,4)$^{+,++}$, Cu1(Ag1)[373] (-4,4,0), Cu1(Ag1)[374] (-4,0,4), Cu1(Ag1)[375] (0,-4,4)$^{++}$, Se2[490] (6,2,2), Se2[491] (2,6,2), Se2[492] (2,2,6), Se2[493] (-6,2,2), Ge[498] (4,4,4), Si[512] (8,0,0) Fig.1. (Here and in tables 1 and 2 the occupied positions are marked by asterisks and empty in various schemes of calculations are marked by cross.)

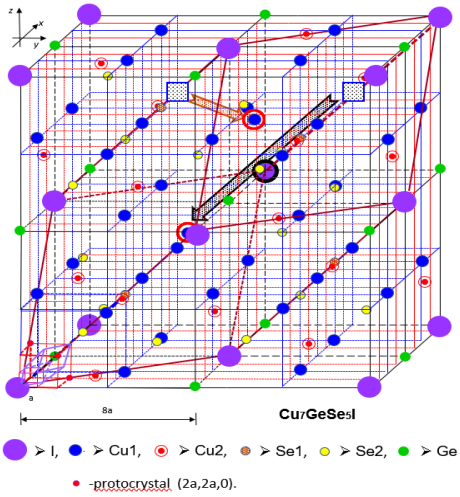



Figure 1. Lattice model ((8a, 8a, 0); (8a, 0.8a); (0.8a, 8a)) in the protocrystal metric (2a, 2a, 0); (2a, 0.2a); (0, 2a, 2a)), the occupied positions are marked. The arrows (yellow) show the transition from the scheme (6 + 1) to the scheme (5 + 2), (gray) from the scheme (5 + 2) to the scheme (4 + 3).

TABLE I. ATOMIC POSITIONS AND OCCUPANCIES OF THE MODEL $Cu_7GeSe_5I$ AND $Ag_7GeSe_5I$ ARGYRODITE STRUCTURES

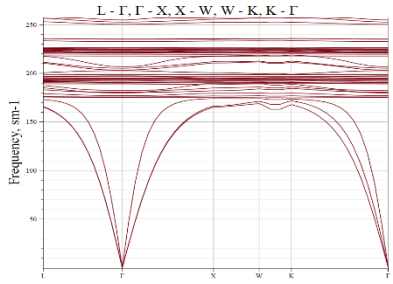
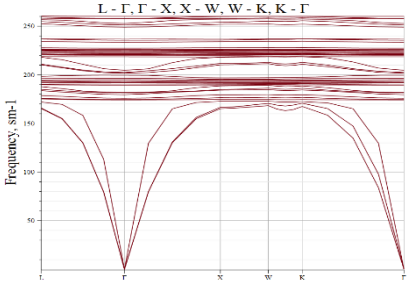
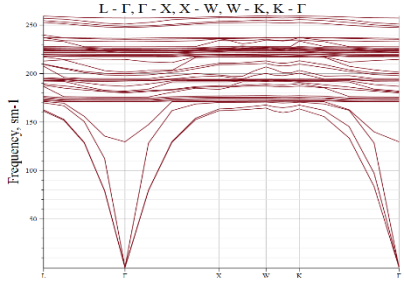
| Atom | Coordinates by [6] | Occu–pancy by [6] | Coordinates by [5] | Occu–pancy by [5] | Model coordinates [this work] | Model occupancy [this work] |
|---|---|---|---|---|---|---|
| Cu1 (Ag1) | (0.02362, 1/4, 1/4) | 0.624 | (0.01747, 0.25, 0.25) | 1.0 | (0, 1/4, 1/4) | 1,5/6*,4/6** |
| Cu2 (Ag2) | (0.01914, 0.30918, 0.30918) | 0.376 | | 0.0 | (0, 5/16, 5/16) | 1/12,2/12*,3/12** |
| I | (0, 0, 0) | 0.989 | (0,0,0) | 1.0 | (0, 0, 0) | 1.0 |
| Se1 | (1/4, 1/4, 1/4) | 0.989 | (1/4, 1/4, 1/4) | 1.0 | (1/4, 1/4, 1/4) | 1.0 |
| Se2 | (0.62183, 0.62183, 0.62183) | 1.0 | (0.62183, 0.62183, 0.62183) | 1.0 | (5/8, 5/8, 5/8) | 1.0 |
| Ge | (1/2,1/2,1/2) | 1.0 | (1/2, 1/2, 1/2) | 1.0 | (1/2, 1/2, 1/2) | 1.0 |

* for calculation in the configuration (5 + 2)
** for calculation in the configuration (4 + 3)

TABLE II. THE ARRAY OF POSITIONS ARRANGED INTO ORBITS AND MODULATION VECTORS IN THE STARS OF $Ag_7GeSe_5I$ AND $Cu_7GeSe_5I$ STRUCTURE WITH (8A,8A,0); (8A,0,8A); (0,8A,8A) SUPERLATTICE OF THE ARGYRODITE FAMILY TO TAKE INTO ACCOUNT THE PARTIAL OCCUPANCY OF CU(AG).

| Atoms and partial population of the orbit | Orbit (position) number | Positions of atoms arranged into orbits | Star number (dimension) | Modulation vectors arranged into stars |
|---|---|---|---|---|
| I | 1(1) | $[0,0,0]$ | 1(1) | $[0,0,0]$ |
| | 2(2-13) | $[a,a,0]$ | 2(12) | $[\pi/8a,\ \pi/8a,\ 0]$ |
| | 3(14-19) | $[2a,0,0]$ | 3(6) | $[\pi/4a,\ 0,\ 0]$ |
| | 4(20-43) | $[2a,a,a]$ | 4(24) | $[\pi/4a,\ \pi/8a,\ \pi/8a]$ |
| | 5(44-55) | $[2a,2a,0]$ | 5(12) | $[\pi/4a,\ \pi/4a,\ 0]$ |
| | 6(56-79) | $[3a,a,0]$ | 6(24) | $[3\pi/8a,\ \pi/8a,\ 0]$ |
| | 7(80-87) | $[2a,2a,2a]$ | 7(8) | $[\pi/4a,\ \pi/4a,\ \pi/4a]$ |
| | 8(88-135) | $[3a,2a,a]$ | 8(48) | $[3\pi/8a,\ \pi/4a,\ \pi/8a]$ |
| | 9(136-141) | $[4a,0,0]$ | 9(6) | $[\pi/2a,\ 0,\ 0]$ |
| Cu2(Ag2)(1/12,2/12*,3/12**) | 10(142-153) | $[3a,3a,0]$ | 10(12) | $[3\pi/8a,\ 3\pi/8a,\ 0]$ |
| | 11(154-177) | $[4a,a,a]$ | 11(24) | $[\pi/2a,\ \pi/8a,\ \pi/8a]$ |
| | 12(178-201) | $[4a,2a,0]$ | 12(24) | $[\pi/2a,\ \pi/4a,\ 0]$ |
| | 13(202-225) | $[3a,3a,2a]$ | 13(24) | $[3\pi/8a,\ 3\pi/8a,\ \pi/4a]$ |
| | 14(226-249) | $[4a,2a,2a]$ | 14(24) | $[\pi/2a,\ \pi/4a,\ \pi/4a]$ |
| | 15(250-297) | $[4a,3a,a]$ | 15(48) | $[\pi/2a,\ 3\pi/8a,\ \pi/8a]$ |
| | 16(298-321) | $[5a,a,0]$ | 16(24) | $[5\pi/8a,\ \pi/8a,\ 0]$ |
| | 17(322-369) | $[5a,2a,a]$ | 17(48) | $[5\pi/8a,\ \pi/4a,\ \pi/8a]$ |
| Cu1(Ag1)(1,5/6*,4/6**) | 18(370-375) | $[4a,4a,0]$ | 18(6) | $[\pi/2a,\ \pi/2a,\ 0]$ |
| | 19(376-399) | $[4a,3a,3a]$ | 19(24) | $[\pi/2a,\ 3\pi/8a,\ 3\pi/8a]$ |
| | 20(400-411) | $[5a,3a,0]$ | 20(12) | $[\overline{3\pi}/8a,\ 3\pi/8a,\ 0]$ |
| | 21(412-423) | $[4a,4a,2a]$ | 21(12) | $[\pi/2a,\ \pi/2a,\ \pi/4a]$ |
| | 22(424-429) | $[6a,0,0]$ | 22(6) | $[3\pi/4a,\ 0,\ 0]$ |
| | 23(430-453) | $[5a,3a,2a]$ | 23(24) | $[\overline{3\pi}/8a,\ 3\pi/8a,\ \pi/4a]$ |
| | 24(454-477) | $[6a,a,a]$ | 24(24) | $[3\pi/4a,\ \pi/8a,\ \pi/8a]$ |
| | 25(478-489) | $[6a,2a,0]$ | 25(12) | $[3\pi/4a,\ \pi/4a,\ 0]$ |
| Se2 | 26(490-497) | $[6a,2a,2a]$ | 26(8) | $[3\pi/4a,\ \pi/4a,\ \pi/4a]$ |
| Se1 | 27(498) | $[4a,4a,4a]$ | 27(1) | $[\pi/2a,\pi/2a,\pi/2a]$ |
| | 28(499) | $[-4a,-4a,-4a]$ | 28(1) | $[\overline{\pi}/2a,\overline{\pi}/2a,\overline{\pi}/2a]$ |
| | 29(500-511) | $[7a,a,0]$ | 29(12) | $[\overline{\pi}/8a,\ \pi/8a,\ 0]$ |
| Si | 30(512) | $[8a,0,0]$ | 30(1) | $[\pi/a,\ 0,\ 0]$ |

+occupancy of the orbit in (5+2) scheme;
++occupancy of the orbit in (6+1) scheme

| $Ag_7GeSe_5I$ | | |
|---|---|---|
| (6+1) | (5+2) | (4+3) |
|  |  |  |
| masses[1] := 127;<br>masses[512] := 72.6;<br>masses[498] := 79;<br>masses[490] := 79;<br>masses[491] := 79;<br>masses[492] := 79;<br>masses[493] := 79;<br>masses[370] := 108;<br>masses[371] := 108;<br>masses[372] := 108;<br>masses[373] := 108;<br>masses[374] := 108;<br>masses[375] := 108;<br>masses[142] := 108; | masses[1] := 127;<br>masses[512] := 72.6;<br>masses[498] := 79;<br>masses[490] := 79;<br>masses[491] := 79;<br>masses[492] := 79;<br>masses[493] := 79;<br>masses[370] := 108;<br>masses[371] := 108;<br>masses[373] := 108;<br>masses[374] := 108;<br>masses[375] := 108;<br>masses[142] := 108;<br>masses[153] := 108. | masses[1] := 127;<br>masses[512] := 72.6;<br>masses[498] := 79;<br>masses[490] := 79;<br>masses[491] := 79;<br>masses[492] := 79;<br>masses[493] := 79;<br>masses[370] := 108;<br>masses[371] := 108;<br>masses[373] := 108;<br>masses[374] := 108;<br>masses[142] := 108;<br>masses[153] := 108.<br>masses[146] := 108 |

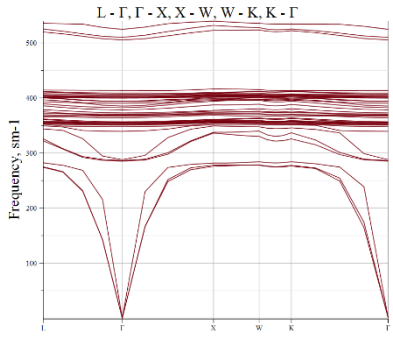
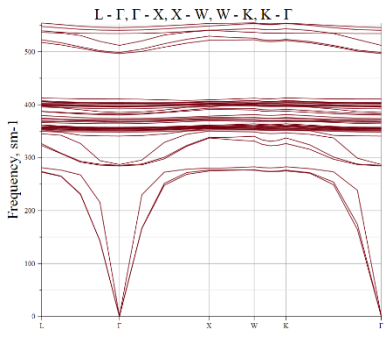
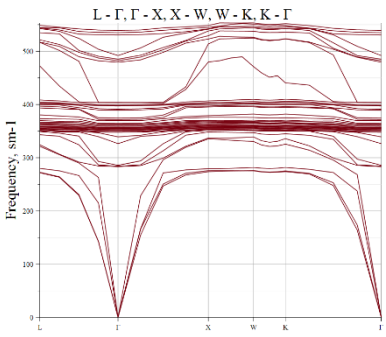
| $Cu_7GeSe_5I$ | | |
|---|---|---|
| (6+1) | (5+2) | (4+3) |
|  |  |  |
| masses[1] := 127;<br>masses[512] := 72.6;<br>masses[498] := 79;<br>masses[490] := 79;<br>masses[491] := 79;<br>masses[492] := 79;<br>masses[493] := 79;<br>masses[370] := 63.5;<br>masses[371] := 63.5;<br>masses[372] := 63.5;<br>masses[373] := 63.5;<br>masses[374] := 63.5;<br>masses[375] := 63.5;<br>masses[142] := 63.5 | masses[1] := 127;<br>masses[512] := 72.6;<br>masses[498] := 79;<br>masses[490] := 79;<br>masses[491] := 79;<br>masses[492] := 79;<br>masses[493] := 79;<br>masses[370] := 63.5;<br>masses[371] := 63.5;<br>masses[373] := 63.5;<br>masses[374] := 63.5;<br>masses[375] := 63.5;<br>masses[142] := 63.5;<br>masses[153] := 63.5. | masses[1] := 127;<br>masses[512] := 72.6;<br>masses[498] := 79;<br>masses[490] := 79;<br>masses[491] := 79;<br>masses[492] := 79;<br>masses[493] := 79;<br>masses[370] := 63.5;<br>masses[371] := 63.5;<br>masses[373] := 63.5;<br>masses[374] := 63.5;<br>masses[142] := 63.5;<br>masses[153] := 63.5;<br>masses[146] := 63.5. |
| powerConstants := [82.1, 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, 0, 10.0, 53, 0.6, 19] | | |

Figure 2. Model phonon dispersion dependences of $Ag_7GeSe_5I$ and $Cu_7GeSe_5I$ crystals, calculated for highly symmetric directions of Brillouin zone, the list of populated positions and the list of values of force constants.

Dynamic matrices of the protocrystal were calculated at 512 points of the Brillouin zone. Modifying the population of crystallographic positions by atoms (in schemes (6 + 1), (5 + 2) and (4 + 3), which cover the average population range of Cu1 and Cu2 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.

The values of the force constants $\alpha_n$ are given in the order of ascending distances between the position of the orbit 1(0, 0, 0) and $n$+1, taking into account all 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 $Ag_7GeSe_5I$, $\alpha_{26n}$ is the force constants describing the interaction at a distance of 4a√3 and equal to 3 N/m, so the others are, correspondingly, powerConstants := Vector[row](28, [15.1, 0, 0, 0, 0, 0.10e-1, 4, 0.10e-1, .6, 1, 0, 0, 0, 0, .7, 0, 3, 7, 0, 0, 0, 0, 2, 0, 0, 0.8e-1, 3, 0, 8.5 (N/m)]. For the $Cu_7GeSe_5I$ compound, the calculations are analogous: powerConstants := [82.1, 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, 0, 2, 0, 0, 10.0, 53, 0.6, 19 (N/m)]. The dispersion dependences for the Γ–L direction of the BZ are shown in Figure 2.

As a result of the model analysis of the structures of $Cu_7GeSe_5I$ and $Ag_7GeSe_5I$ taking into account the occupancy of the orbit of the Cu2(Ag2) 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 of the $Cu_7GeSe_5I$ and $Ag_7GeSe_5I$ crystals was observed, which is caused by the change of the corresponding mass characteristics of the Cu and Ag atoms and by a certain expected correlation between the power constants. The results of the 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 [8]. The wide frequency ranges of values obtained in the present work can indicate the effective possibility of their changes by changing the occupancy of the Cu(Ag) atoms (*i.e.* by a "jump" of atoms between the considered orbits), which is accompanied by the high ionic conductivity in the superionic $Cu_7GeSe_5I$ and $Ag_7GeSe_5I$ crystals.

## IV. Conclusions

As a result of the model analysis of the structures of $Cu_7GeSe_5I$ and $Ag_7GeSe_5I$ taking into account the different schemes of occupancy of the orbit of the Cu(Ag) atom 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 is 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, is obtain. Note the satisfactory coincidence of the range of calculated frequencies with the experimental values of frequencies 150-350 $cm^{-1}$ at the Γ point [9]. 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 optical frequencies changes, 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 superionic phase of crystals which in turn can contribute to high ionic conductivity in the superionic phase of crystals $Cu_7GeSe_5I$ and $Ag_7GeSe_5I$ (by a "jump" of atoms between the considered orbits). At the same time, the increase in the deviation from the classical disintegration of atoms in cubic syngony crystals 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, note that the preference in this analysis can be given to the system $Ag_7GeSe_5I$ compared to $Cu_7GeSe_5I$.

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