Model phonon spectra and densities of states of crystals Mo_3Ge, Nb_3Ge and V_3Ge

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The effectiveness of the combination of the concept of superspace symmetry [1,2] and ideas of the lattice model [3] for calculation of model phonon spectra of complex crystal formations [4-6] has been shown. (3+3)-dimensional bases, sets of modulation vectors, modulation functions, generalized dynamic matrices and ($4a\times4a\times4a$) lattice model for describing the crystal structure and calculations of model phonon spectra and densities of states of Mo_3Ge, Nb_3Ge and V_3Ge structures for various combinations of force constants have been presented.

Representatives of the A-15 family are interesting as the most high-temperature superconductors. The progenitor of this family is aluminum niobium Nb_3Al [7], a typical superconductor with the structure A-15 (cubic structure of type β-W with the space group Pm3n No. 200. The simple cubic unit cell contains 8 atoms in the positions ([0,0,0], [1/2,1/2,1/2],[x,1/2,0],[-x,1/2,0],[0,x,1/2],[0.-x ,1/2],[1/2,0,x],[1/2,0,-x]) where x=1/4. It is convenient to set all these positions in the lattice model of order 64. For their generation the (3+3)-dimensional direct and inverse bases were used [4-6]:

The calculated model phonon spectra and densities of states of the indicated representatives of this family with using the methodology [1, 4-6] are illustrated in Fig. 1.

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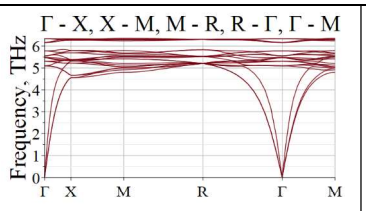
<td> 
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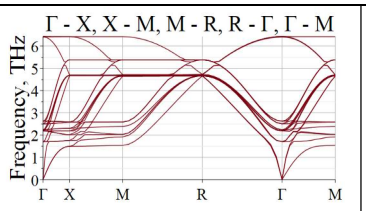
<td> 
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<td>Mo_6Ge_2 (95.94,72.6) powerConstants: = Vector[row](10, [0, 0, 0, 10.9.10,01.10, 9, 0, 0, 0, 0])</td>
<td>Mo_6Ge_2 (95.94,72.6), powerConstants: = Vector[row](10, [0, 0, 0, 60.9.1,0.1,05, 0, 0, 0]),</td>
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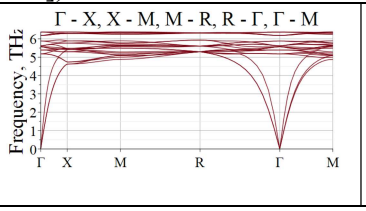
<td> 
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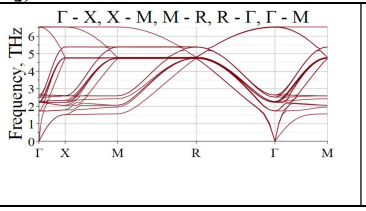
<td> 
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<td>Nb_6Ge_2 (92,9,72.6). powerConstants: = Vector[row](10, [0, 0, 0, 10.9.10,01.10, 9, 0, 0, 0])</td>
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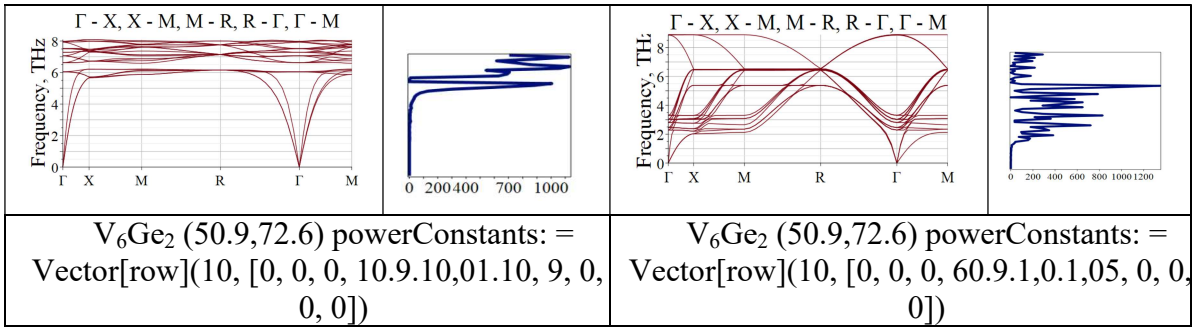

V_6Ge_2 (50.9,72.6) powerConstants: = Vector[row](10, [0, 0, 0, 10.9.10,01.10, 9, 0, 0, 0])	V_6Ge_2 (50.9,72.6) powerConstants: = Vector[row](10, [0, 0, 0, 60.9.1,0.1,05, 0, 0, 0])

Fig. 1. Model phonon dispersion dependences and densities of phonon states of Mo_3Ge, Nb_3Sn and V_3Ge crystals calculated for highly symmetric directions of the Brillouin zone in schemes with different combinations of force constant values.

The values of the force constants α_l are given in order of increasing the distance between the orbital positions 1(0,0,0) and l+1, while all possible variants of the distances between pairs of positions occupied by atoms were taken into account. The force constants were chosen in the equidistant approximation. For example, for the Nb_3Sn structure, the power constant α_4, which describes the interaction at a distance of 2*a*, is equal to 10.9 n/m, and all others are equal, respectively, to (powerConstants: = Vector[row](10,[0,0,0,10.9.10,01.10 ,9,0,0,0,0]). Two identical combinations of force constants were chosen for all the investigated crystals.

The resulting model calculations reflect the modification of phonon spectra exclusively depending on the mass characteristics of metal atoms. It is shown that by choosing the certain combinations of force constant values, mainly α_4, α_5 and α_6, it is possible to obtain phonon spectra with optical frequencies within the range of 150 to 240 cm^{-1} (for Nb_3Sn crystals, it correlates with the experimental data [7]). At the same time, the distribution of densities of phonon states is significantly different. We note the proximity of the ranges of high-frequency optical branches for a number of crystals and significant difference in the values for low-frequency and especially acoustic branches.

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