Vacancy-suppressed lattice conductivity of high-ZT $\text{In}_4\text{Se}_{3-x}$

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Vacancy-Suppressed Lattice Conductivity of high-$ZT$ In$_x$Se$_{3-x}$

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Anomalous, vacancy-induced anisotropic thermal conductivity is one of the important properties in the recently discovered high-$ZT$ In$_x$Se$_{3-x}$ compound. In this work, the lattice thermal conductivity of In$_x$Se$_{3-x}$ is investigated using equilibrium molecular dynamics simulation, the point-defect model, and ab initio calculations. The charge density wave (CDW) induced by quasi one-dimensional lattice distortion (Peierls distortion) enhances the power factor $\sigma T$ and lowers lattice conductivity. This suggests a new direction in search for high-$ZT$ TE materials, beyond Bi$_2$Te$_3$ and PbTe. Recently, experiments using chemical doping and nanostructures have aimed at further increasing $ZT$ of In$_x$Se$_{3-x}$, and there has been theoretical investigation of high-$ZT$ In$_x$Se$_{3-x}$ using the electronic structure calculations.

The electronic properties such as $S$ and $\sigma_x$ of In$_x$Se$_{3-x}$ are well investigated by the combination of Boltzmann transport equation and ab initio band structure calculations. Using a simple rigid-band and constant relaxation time approximation, the calculated power factor is in good agreement with the experimental results. Also the electronic structure calculation predicts the enhancement of power factor with electron doping, which is correctly realized in Cl-doped structure (In$_x$Se$_{3-x}$Cl$_{0.03}$). Thermal conductivity, however, is not well described by electronic structure calculations because the lattice (phonon) contribution is dominate over electric thermal conductivity. For accurate prediction of $ZT$ in In$_x$Se$_{3-x}$, the lattice dynamics and phonon scattering should be investigated.

The orthorhombic lattice structure (space group $Pnma$) of In$_x$Se$_3$ contains warped $b$-$c$ plane layers which are stacked along $a$-axis (Fig. 1(a)). Within the layer, three distinct In-Se-In zigzag chains are aligned along the $c$-axis (Fig. 1(b)), indicated by black, blue, and red lines. For all the chains, the In atoms are connected with Se atoms by an ionic-covalent bond. The warped layers are stacked with weak inter-molecular bond along $a$-direction. Most of layered compounds usually show higher in-plane thermal conductivity than that of cross-plane because of the strong inter-atomic bonding. However, experimental thermal conductivity of In$_x$Se$_{3-x}$ shows unusual behavior; the $b$-$c$ plane thermal conductivity is much lower than that in the $a$-$b$ plane. Because high In$_x$Se$_{3-x}$ $ZT$ is closely related to the low $b$-$c$ plane thermal conductivity, it will be important to explain this unusual anisotropy in the lattice thermal conductivity.

FIG. 1. (Color online) Crystal structure of In$_x$Se$_3$. (a) Perspective view of the $a$-$b$ plane. Gray and yellow spheres represent In and Se atoms, respectively. (b) The structure contains three distinct In-Se-In chains along $c$-axis; blue, black and red lines indicate In1-Se1, In2-Se2, In3-Se3 chains, respectively. (c) Crystal structure of In$_x$Se$_{3-x}$, containing Se3 vacancy.

The high-temperature lattice conductivity of semiconductors has been explained with the simple analytical approach, point-defect model, first developed by Klemens and Callaway and
von Baeyer. This model, derived from the consideration of phonon scattering processes to the thermal resistance, has been successfully applied to thermal transport in a variety of TE materials. Various crystal imperfections (e.g., vacancies, interstitial atoms, and site substitution) can be considered as point-defects to reduce the lattice conductivity due to the phonon scatterings with mass contrast, atomic displacement, and/or local strain induced by the defect. In In4Se3, the randomly distributed Se vacancies are expected to scatter phonons. However, the point-defect model has not commonly applied to highly anisotropic system such as In4Se3.

Here using molecular dynamics (MD) simulation, the point-defect model, and ab initio calculations, we investigate the lattice conductivity of In4Se3 to (i) predict the lattice conductivity tensor of In4Se3, and (ii) explain the origin of its unusual anisotropy. Our results show the lattice conductivity along the chain direction is sensitively suppressed with the Se-deficient In4Se3 structure. On the other hand, the Se vacancy moderately suppresses the lattice conductivity perpendicular to the chain. So the low in-plane (b-c plane) lattice conductivity in In4Se3 is consistent with the experimental observations.

**METHODS AND MODELS**

**Ab initio calculations**

In order to determine the preference of Se vacancy sites in In4Se3, we construct a hypothetical crystal structure and remove one Se atom of In4Se3 at the Se1, or Se2, or Se3 sites, respectively. In our density functional calculations of In4Se3, we employed the frozen-core projector augmented wave method encoded in the Vienna ab initio simulation package, and the generalized-gradient approximation of Perdew, Burke and Ernzerhof for the exchange-correlation functional with the plane-wave-cut-off energy of 450 eV and a set of 80 k-point in the irreducible Brillouin zone. The threshold for the self-consistent-field convergence of the total electronic energy was 10⁻⁶ eV.

**Interatomic potentials**

We construct the classical interatomic potentials for In4Se3 developed on the basis of experimental lattice properties by using GULP (general utility lattice program). The classical Morse and three-cosine interatomic potentials were fitted to the elastic constants. The fitted interatomic potentials undergo the GULP optimization of the crystal structure under constant pressure. In the fitting process, we calculate the elastic constants Cijkl and compare them with the experimental values. The resulting Cijkl are listed in Table 1 and compared with the experiments. Our results show better agreement with experiments than those in the previous theoretical results with only central two-body interactions. The resulting optimized potential parameters are listed in Table 2.

**Lattice conductivity from MD simulations**

The high-temperature (T > 0.1TD, where TD is the Debye temperature) lattice conductivity tensor Kx is dominated by phonon-phonon scattering and is calculated using equilibrium MD and the Green-Kubo heat current autocorrelation function (HCACF) decay

\[
K_i = \frac{V}{k_B T} \int_0^\infty \langle q(t)q(0) \rangle dt.
\]

where \(k_B\) is the Boltzmann constant, \(V\) is the volume of the MD simulation, \(\langle q(t)q(0) \rangle\) is the HCACF tensor, and the heat current vector \(q\) is

\[
q = \frac{1}{V} \frac{d}{dt} \sum_i \vec{v}_i.
\]

**Table 1. Comparison of calculated elastic constants Cijkl (in GPa) of In4Se3 compared with experiments and other theoretical results.**

<table>
<thead>
<tr>
<th>C11</th>
<th>C12</th>
<th>C13</th>
<th>C22</th>
<th>C23</th>
<th>C33</th>
<th>C44</th>
<th>C55</th>
<th>C66</th>
</tr>
</thead>
<tbody>
<tr>
<td>38.2</td>
<td>10.8</td>
<td>30.4</td>
<td>66.5</td>
<td>22.4</td>
<td>64.3</td>
<td>16.6</td>
<td>26.6</td>
<td>19.0</td>
</tr>
<tr>
<td>49.8</td>
<td>15.6</td>
<td>26.1</td>
<td>58.9</td>
<td>21.7</td>
<td>52.2</td>
<td>18.7</td>
<td>33.0</td>
<td>16.1</td>
</tr>
<tr>
<td>36.4</td>
<td>13.7</td>
<td>22.4</td>
<td>68.9</td>
<td>24.9</td>
<td>62.0</td>
<td>20.5</td>
<td>32.5</td>
<td>22.7</td>
</tr>
</tbody>
</table>

**Table 2. The two- and three-body interatomic potential parameters (excluding the electrostatic interactions) for In4Se3. Morse potential \(v(r) = [1 - \exp(-a(r - r_c))]^2 - 1\) for two-body, and three cosine \([v(r)\cos\theta - \cos\theta]^2/2\) for three-body interactions. Here, \(r\) and \(\theta\) are interatomic separation distance and bond angle.**

<table>
<thead>
<tr>
<th>Interaction</th>
<th>Parameters</th>
<th>Interaction</th>
<th>Parameters</th>
</tr>
</thead>
<tbody>
<tr>
<td>Two-body</td>
<td>(v_0 (eV))</td>
<td>(a (\AA^{-1}))</td>
<td>(r_c (\AA))</td>
</tr>
<tr>
<td>In1-Se1</td>
<td>1.83</td>
<td>1.67</td>
<td>2.69</td>
</tr>
<tr>
<td>In2-Se2</td>
<td>2.80</td>
<td></td>
<td></td>
</tr>
<tr>
<td>In3-Se3</td>
<td>2.63</td>
<td></td>
<td></td>
</tr>
<tr>
<td>In1-Se2</td>
<td>1.29</td>
<td>1.27</td>
<td>2.62</td>
</tr>
<tr>
<td>In3-Se2</td>
<td>2.71</td>
<td></td>
<td></td>
</tr>
<tr>
<td>In2-In3</td>
<td>1.44</td>
<td>1.32</td>
<td>2.75</td>
</tr>
<tr>
<td>In1-In2</td>
<td>2.78</td>
<td></td>
<td></td>
</tr>
<tr>
<td>In2-Se3</td>
<td>0.96</td>
<td>1.19</td>
<td>3.43</td>
</tr>
<tr>
<td>In3-In3</td>
<td>3.69</td>
<td></td>
<td></td>
</tr>
<tr>
<td>In4-In4</td>
<td>0.9</td>
<td>1.3</td>
<td>3.44</td>
</tr>
<tr>
<td>In4-In2</td>
<td>3.79</td>
<td></td>
<td></td>
</tr>
<tr>
<td>In4-Se3</td>
<td>0.7</td>
<td>0.45</td>
<td>2.97</td>
</tr>
<tr>
<td>In4-Se2</td>
<td>0.6</td>
<td>1.01</td>
<td>3.16</td>
</tr>
<tr>
<td>In4-Se1</td>
<td>0.5</td>
<td>1.03</td>
<td>3.39</td>
</tr>
<tr>
<td>In1-Se1</td>
<td>101.1</td>
<td></td>
<td></td>
</tr>
<tr>
<td>In1-Se3</td>
<td>101.3</td>
<td></td>
<td></td>
</tr>
<tr>
<td>In2-Se2</td>
<td>101.3</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
where \( \mathbf{r} \) and \( E \) are the position vector and the total energy of the particle (atom), respectively. After checking the size effect on the result of MD simulation, the simulations are performed in a 3 × 3 × 12 orthorhombic unit cells with 3024 (3024 – 432x for \( \text{In}_4\text{Se}_{3-x} \)) atoms. The temperature ranges from 300 to 700 K, with 100 K interval with a time step of 20 fs. The Verlet leapfrog algorithm with the Nose-Hoover thermostat and the Berendsen barostat are used in the NPT ensemble for 200 ps and then in NVE for 100 ps to reach equilibrium. Then 2000 ps raw heat current data are obtained for the calculation of HCACF. The resulting HCACF is then directly integrated and \( K_p \) is averaged in the smoothened converged region.

**Point-defect model of lattice conductivity**

In order to analyse the change of \( K_p \), as a function of Se vacancy concentration \((x)\) and temperature, we use the analytical treatment, point-defect model. Starting with \( K_p \) of \( \text{In}_4\text{Se}_x \) \((x = 0)\), which are dominated by the phonon-phonon scattering parameter \( n \), we take the point-defect scattering for the compound with vacancies.

From the Matthiessen rule, the isotropic overall \( k_{p,d} \), with the inclusion of the point-defect scattering \( k_{p,d} \), is \( 1/k_{p,d}(T) = 1/k_{p,0}(T) + 1/k_{p,d}(T) \). Here \( k_{p,0}(T) \) is obtained from our MD results. For the description of \( k_{p,d} \), we start with the mass fluctuation scattering parameter \( \Gamma \), which is given by

\[
\Gamma = \pi (1 - \chi) \left( \frac{\Delta M}{M} \right),
\]

where \( M \) is the average mass of compound \( \text{In}_4\text{Se}_{3-x} \). The lattice conductivity limited by the point-defect scattering \( k_{p,d} \) is

\[
k_{p,d} = \frac{k_B}{4\pi M_{p,A} (\omega_{CT})^{1/2}},
\]

where \( k_B \) is the Boltzmann constant, \( \omega_{CT} \) is the relaxation time for interphonon scattering including Normal (N-) and Umklapp (U-) processes. Here \( \omega_{CT} \) can be estimated from the pure \( \text{In}_4\text{Se}_2 \) at 300 K using

\[
\omega_{CT} = \frac{(6n)^{1/3}}{2\pi^{4/3}} k_B \frac{\alpha_i}{k_{p,0}},
\]

where \( n \) is the atomic number density. The parameter \( \alpha_i \) is the coefficient for the Rayleigh point-defect scattering rate, given by

\[
\alpha_i = \frac{V'_c \Gamma}{4\pi M_{p,A}^{1/2}},
\]

where \( V'_c \) is the unit-cell volume and \( u_{p,A} \) is the average phonon group velocity.

**RESULTS AND DISCUSSION**

**Se vacancy formation**

Table 3 shows relative energy of each Se vacancy model obtained from \textit{ab initio} calculations, and shows that Se3 is the most preferable site for the formation of the Se vacancy. The result is reasonable considering the bonding structures around the Se ions. As shown in Fig. 1(a), Se3 has only two nearest neighbors while Se1 and Se2 have three nearest neighbors with ionic-covalent bonding with In atoms. Because Se1 and Se2 are very important in sustaining stable \( b-c \) plane layer, the Se3 is the most probable vacancy site. So in the MD simulations, we use only Se3 vacancy for \( \text{In}_4\text{Se}_{3-x} \) structure. To avoid the repetition of the Se3 vacancies along the \( c \)-direction, we use a 1 × 1 × 4 supercell to distribute the Se3 vacancies randomly. We also considered several other structure orders with different Se3 vacancy site and the results showed consistent anisotropic behavior of the lattice conductivity. To fully examine all possible Se3 sites, a much larger supercell is required (computation is very extensive) and that was considered outside the scope of the current study.

<table>
<thead>
<tr>
<th>Site</th>
<th>Se1</th>
<th>Se2</th>
<th>Se3</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Delta E ) (meV)</td>
<td>131.92</td>
<td>65.20</td>
<td>0.00</td>
</tr>
</tbody>
</table>

**Lattice conductivity of \( \text{In}_4\text{Se}_{3-x} \)**

Our equilibrium MD based lattice conductivity results for \( \text{In}_4\text{Se}_x \) show the expected temperature dependence as shown in Fig. 2(a). For \( x = 0 \), the \( c \)-direction lattice conductivity is much larger than that in other directions for all temperatures. This makes the \( b-c \) plane lattice conductivity larger than the \( a-b \) plane, which we expect from the lattice and elastic constants. For \( x = 0.5 \), however, the \( c \)-direction lattice conductivity is noticeably reduced, while the \( a \)- and \( b \)-direction lattice conductivity show much smaller suppression (Fig. 2(a), dashed lines). In Fig. 2(a), we remove standard error bars because of complexity, which is allowed in 10–20% range. The error is decreased as temperature and Se vacancy increases. Our results are well consistent with the experimental observation that \( a-b \) plane thermal conductivity is larger than the \( b-c \) plane thermal conductivity in \( \text{In}_4\text{Se}_{2.5} \) (Fig. 2(b)).
exponential functions, i.e., a fast decaying short-range and a slow decaying long-range decay.\(^{14,21,22}\) The long-range acoustic lattice conductivity has a strong temperature dependence (Fig. 2(c), rectangular symbol) and dominates the lattice conductivity, while the short-range acoustic and optical lattice conductivities are relatively small and independent of temperature and direction (i.e., \(k_\text{p,a,b} = 0.25\) and \(k_\text{p,o} = 0.08 \text{ W/m-K}\)). For \(\text{In}_4\text{Se}_3\) \((x = 0.5)\), this phonon transport decomposition shows suppression of the long-range acoustic transport mainly, while the temperature-independent, short-range acoustic and optical transports remain almost same (Fig. 2(d)). So we confirmed only the long-range acoustic phonon is suppressed with Se vacancy which will be discussed later.

To verify our MD lattice conductivity we compare it with the directional Slack relation which represent the long-range phonon conductivity\(^{23,26}\), i.e.,

\[
k_{a,b,c} = \frac{3.1 \times 10^{10} \left(M/N^3\right) \Delta T^{3.4}}{T_\text{D,a,b,c}}, \quad \alpha = a, b, c.
\]  

(8)

Here, \(\langle M \rangle\) is the mean atomic weight of the atoms in the primitive cell, \(\delta\) is the average volume per atom, \(N\) is the number of atoms in a primitive cell, \(T_\text{D,a}\) is the high-temperature Debye temperature, and \(\gamma_{\alpha,a}\) is the directional Grüneisen parameter (indicative of the bonding character in the lattice\(^{29}\)) defined as

\[
\gamma_{\alpha,a} = \frac{\sum_{\nu} d \ln \omega_{\nu}(\mathbf{K}) \ln \nu}{\sum_{\nu} d \ln \nu}, \quad \alpha = a, b, c.
\]

(9)

where, \(\omega_{\nu}(\mathbf{K})\) is phonon frequency. Directional Debye temperature and Grüneisen parameter, which are obtained from the MD results using the interatomic potentials, are listed in Table 4. Due to the strong bond along the \(c\)-direction, \(T_{\text{D,c}}\) has the lowest value. Using these results, the directional long-range acoustic lattice conductivity calculated by eq 8 is also shown in Fig. 2(c). The directional Slack results are in reasonable agreement with the decomposed MD results for \(\text{In}_4\text{Se}_3\) \((x = 0)\).

### Anisotropic Reduction in lattice conductivity of \(\text{In}_4\text{Se}_3\)

We investigated the unusual anisotropic behavior of \(\text{In}_4\text{Se}_3\) and we compare directional lattice conductivities with respect to Se vacancy \(x\) in Fig. 3 at 300 K. For \(\text{In}_4\text{Se}_3\) \((x = 0)\), the \(c\)-direction lattice conductivity is the largest which makes the \(b\)-plane conductivity larger than that in the \(a\)-\(b\) plane. With Se vacancy, the \(c\)-direction conductivity is reduced a lot more than those in the \(a\)-\(b\) plane. The point-defect model considers generally uses the no-defect phonon velocities, the \(a\)- and \(b\)-directional conductivities are well described by the point-defect model. However, the \(c\)-direction conductivity is suppressed more than that predicted by the point-defect model. The changes in the phonon velocity with the Se vacancy along each direction are summarized in Table 4. While the phonon velocity for \(a\)- and \(b\)-directions decrease by 11% and 5% for \(x = 0.5\), the \(c\)-direction shows 17%.

We also analysed the effect of Se vacancy with the point-defect model. For calculation of the lattice conductivity with eq 4, we use the reported and calculated thermodynamic/phonon properties at room temperature summarized in Table 4. These analytical model results for the point-defect scattering model are compared with the MD results in Fig. 3. The model predictions along the \(a\)- and \(b\)-directions are in good agreement with the MD results over the range of vacancy concentration and temperature. Hence, we conclude that the isotropic point-defect scattering including the mass fluctuation accurately predicts the \(k_\text{p,c}\) reduction in \(\text{In}_4\text{Se}_3\) in these directions. Along \(c\)-direction, however, the isotropic point-defect model does not predict the significant suppression of \(k_{p,a}\) suggesting the phonon softening due to the bond softening is significantly directional in this material. This anisotropy results in an extra 50% reduction of \(k_{p,a}\) over what is predicted by the isotropic point-defect model.

### Origin of vacancy-induced anisotropy in lattice conductivity

To explain the origin of anisotropic effect of vacancy on the lattice conductivity, we calculate the phonon dispersion curves for \(\text{In}_4\text{Se}_3\) using the obtained interatomic potentials. Figure 4(a) shows the total phonon dispersion for each direction in the \(\text{In}_4\text{Se}_3\) structure. The dispersion is well matched with that reported in Ref. [7]. With Se vacancy (Fig. 4(b)), flat dispersion curve around 1 THz appears to contribute to the acoustic phonon dispersion along the \(c\)-direction. Along \(a\)- and \(b\)-directions, there is negligible change in the acoustic phonon dispersion. As a result, the phonon velocity along \(c\)-direction is significantly suppressed with the Se vacancy, while other directions are showing small changes. Because the point-defect model considers generally uses the no-defect phonon velocities, the \(a\)- and \(b\)-directional conductivities are well described by the point-defect model. However, the \(c\)-direction conductivity is suppressed more than that predicted by the point-defect model. The changes in the phonon velocity with the Se vacancy along each direction are summarized in Table 4. While the phonon velocity for \(a\)- and \(b\)-directions decrease by 11% and 5% for \(x = 0.5\), the \(c\)-direction shows 17%.

The suppressed phonon velocity along \(c\)-direction can be understood with the crystal structure containing the In-Se-In chains along \(c\)-direction as shown in the Fig. 1(b). The bundle of atomic chains along \(c\)-direction makes for high lattice conductivity because of high phonon speed along that direction in the absence of vacancy. The bundlings along \(a\)- and \(b\)-directions have more complicated structures compared with the \(c\)-direction. With Se vacancy, the conducting channels of In-Se-In chains are broken. The chain breaking is well described by the charge density distributions in \(\text{In}_4\text{Se}_3\) and \(\text{In}_4\text{Se}_{2.5}\) lattice as shown in Fig. 5(a) and 5(b). In Fig. 5(a), the charge density distribution shows strong bonding along In-Se-In chains, which give high phonon transport of \(\text{In}_4\text{Se}_3\) compound. When the strong In-Se-In bonding is broken (Fig. 5(b)), the disconnected charge density reduces phonon transport, especially along the \(c\).

### Table 4. Calculated directional Debye temperatures, Grüneisen parameters, and average phonon group velocities of \(\text{In}_4\text{Se}_{3-x}\)

<table>
<thead>
<tr>
<th>Directions ((\alpha))</th>
<th>(T_{\text{D,a}}) (K)</th>
<th>(\gamma_{\text{G,a}})</th>
<th>(u_{p,g,A,a}) (m/s, (x = 0))</th>
<th>(u_{p,g,A,a}) (m/s, (x = 0.25))</th>
<th>(u_{p,g,A,a}) (m/s, (x = 0.5))</th>
</tr>
</thead>
<tbody>
<tr>
<td>(a)</td>
<td>226</td>
<td>1.94</td>
<td>2286</td>
<td>2186</td>
<td>2029</td>
</tr>
<tr>
<td>(b)</td>
<td>226</td>
<td>1.81</td>
<td>2287</td>
<td>2239</td>
<td>2183</td>
</tr>
<tr>
<td>(c)</td>
<td>239</td>
<td>1.56</td>
<td>2311</td>
<td>2145</td>
<td>1922</td>
</tr>
<tr>
<td>Ref. [3]</td>
<td>260</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

FIG. 3. (Color online) Variation of the directional lattice conductivity of \(\text{In}_4\text{Se}_{3-x}\) as a function of vacancy at 300 K. The calculated MD results (solid lines) are compared with point-defect model (dashed lines).
FIG. 4. (Color online) Phonon dispersion curves and density of state of (a) In$_4$Se$_3$, and (b) In$_4$Se$_{2.75}$. [1,0,0], [0,1,0], and [0,0,1] indicate the a-, b-, and c-directions in the structure, respectively.

Also, the CDW induced structural distortion, which is argued in Ref. [1], could break the quasi-one-dimensional chains to suppress the phonon transport. So the In-Se-In chain and the vacancy in the chain are the key elements to explain the anisotropic lattice conductivity in In$_4$Se$_{3-x}$ compound.

FIG. 5. (Color online) Charge density distributions in (a) In$_4$Se$_3$, (b) In$_4$Se$_{2.9}$ lattice.

CONCLUSIONS

In summary, we investigated the anisotropic behaviour of lattice conductivity for In$_4$Se$_{3-x}$ compound using various theoretical works. The interatomic potentials are developed for MD simulation of and lattice conductivity prediction of In$_4$Se$_{3-x}$, and the good agreement of the calculated elastic constants with the experiments indicates that the proposed force fields are suitable for both harmonic and anharmonic behaviours of In$_4$Se$_3$. Using developed interatomic potential, the temperature dependence of directional lattice conductivities has been calculated in a temperature range from 300 to 700 K with and without Se vacancy. The results reproduce well the experimental observations of lattice conductivities with Se vacancy. Without Se vacancy, c-direction conductivity is the highest due to strong bonding along In-Se-In chain, while it is suppressed even below a- and b-direction conductivity with Se vacancy. The calculated phonon dispersion and the charge density distribution also support the anisotropic changes of lattice conductivity.

We show that the Se vacancy in the quasi-one-dimensional In-Se-In chain has dominant role in the suppression of long-range acoustic phonon transport and very low lattice conductivity along the chain direction. Our results could give a new direction for finding good TE materials in controlling the lattice conductivity.

ACKNOWLEDGMENTS

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