Thermal conductivity of CaF$_2$ at high pressure

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We study the thermal transport properties of three CaF$_2$ polymorphs up to a pressure of 30 GPa using first-principle calculations and an interatomic potential based on machine learning. The lattice thermal conductivity $\kappa$ is computed by iteratively solving the linearized Boltzmann transport equation (BTE) and by taking into account three-phonon scattering. Overall, $\kappa$ increases nearly linearly with pressure, and we show that the recently discovered $\delta$-phase with $P62m$ symmetry and the previously known $\gamma$-CaF$_2$ high-pressure phase have significantly lower lattice thermal conductivities than the ambient-thermodynamic cubic fluorite ($Fm\bar{3}m$) structure. We argue that the lower $\kappa$ of these two high-pressure phases stems mainly due to a lower contribution of acoustic modes to $\kappa$ as a result of their small group velocities. We further show that the phonon mean free paths are very short for the $P62m$ and $Pnma$ structures at high temperatures, and resort to the Cahill-Pohl model to assess the lower limit of thermal conductivity in these domains.

I. INTRODUCTION

Calcium fluoride (CaF$_2$) has a variety of technological applications due to its remarkable optical properties and its high thermal stability.$^{1,2}$ At ambient conditions, $\alpha$-CaF$_2$ crystallizes in the cubic fluorite structure with $Fm\bar{3}m$ symmetry. In this structure, CaF$_2$ exhibits a super-wide band gap of 12 eV with excellent light transmission over a wide spectrum, and a high laser damage threshold. These properties render CaF$_2$ an ideal candidate for optical windows, main lens substrates in large scale semiconductor micro-lithography systems, and photo-detectors$^{3,4}$.

Cubic CaF$_2$ undergoes a sequence of structural phase transitions at increased pressures.$^{5,6}$ Above 8–10 GPa, CaF$_2$ transforms to the denser orthorhombic cotunnite $\gamma$-phase with $Pnma$ symmetry, accompanied by an increased coordination number of Ca from 8 to 9. X-ray diffraction and Raman spectroscopy have shown that this high-pressure phase is stable up to 49 GPa at room temperature.$^{13,15}$ As pressure increases further, the stability of $\gamma$-CaF$_2$ decreases, and above 72 GPa, a further transition occurs to a hexagonal $P6_3/mmc$ phase.$^{10}$

In addition to these experimentally observed low-temperature high-pressure phases, high-temperature modifications thereof have been studied predominantly using computational models. Using $ab$ initio structural searches, Nelson et al. recently proposed a hypothetical structure with $P62m$ symmetry as a high-temperature polymorph of $\gamma$-CaF$_2$, referred to as $\delta$-CaF$_2$. Similar to its ambient-pressure counterpart, $\delta$-CaF$_2$ is predicted to undergo a transition to a superionic phase with bcc structure at temperatures exceeding $\approx$ 2500 K at 20 GPa.

Despite these theoretical studies, little is known about the high-pressure behavior of the thermal transport properties in CaF$_2$ polymorphs. At ambient pressure, the lattice thermal conductivity of $\alpha$-CaF$_2$ has been studied both through experiments and computations. In two separate early experiments in 1957 and 1960, the near room-temperature value of the lattice thermal conductivity was measured to be 5.5$^{22}$ and 9.1$^{27}$ Wm$^{-1}$K$^{-1}$, respectively. Later, Slack$^{28}$ reported a value of 11.69 Wm$^{-1}$K$^{-1}$ in 1961. Theoretical room-temperature values from simulations have been predicted in the range of 7.0 and 8.6 Wm$^{-1}$K$^{-1}$. To the best of our knowledge, the only work on the pressure dependence of $\kappa$ in $\alpha$-CaF$_2$ was reported $9.7 < \kappa < 10.9$ Wm$^{-1}$K$^{-1}$, measured using a dynamic two-strip method at room temperature in a narrow pressure range of 0.1 to 1.0 GPa.$^{27}$

In this work, we study the thermal conductivity of the $\alpha$, $\gamma$, and $\delta$ phases of CaF$_2$ as a function of pressure in the range of 0–30 GPa. To alleviate the computational burden of $ab$ initio calculations, we resort to training an efficient machine learning interatomic potential to accelerate the assessment of the lattice thermal conductivity $\kappa$. We show that the value of $\kappa$ for the $\gamma$-CaF$_2$ and $\delta$-CaF$_2$ phases are lower than that of the $\alpha$ phase across the whole pressure domain. In particular, the extremely small phonon mean-free-paths in these two phases leads to a potential break-down of the Boltzmann transport equation (BTE). Hence, we assess the validity of the BTE results based on the amorphous limit using the Cahill-Pohl model and draw the associated temperature-pressure transition boundary.

II. METHODS

A. Interatomic Potential

We use CENT, a neural-network-based interatomic potential, that takes into account charge transfers to model the ionic bonding in CaF$_2$. The construction of the CaF$_2$ CENT potential is discussed in detail elsewhere.$^{29}$ and we employ its implementation in the FLAME package.$^{30–32}$ The particular parametrization of our CENT potential has been used elsewhere to obtain physical properties of CaF$_2$ and to study surface morphologies.
of CaF$_2$.

B. Density Functional Theory

Structural relaxations and single-point total energy calculations were performed with density functional theory (DFT) calculations at selected pressures, 2, 10, and 30 GPa. We used the plane-wave Quantum ESPRESSO simulation package in conjunction with the Perdew-Burke-Ernzerhof (PBE) parametrization of the exchange-correlation functional and ultrasoft pseudopotentials. The wave functions and electron densities were expanded with a plane wave basis set up to a kinetic energy cutoff of 45 Ry and 540 Ry, respectively. The Brillouin zone was sampled using a Monkhorst-Pack k-points mesh of 50 \times 50 \times 50. Structural relaxations (one longitudinal and two transverse acoustic branches) were calculated by applying the Pearson deviation coefficients incorporated in ShengBTE. The so-called proportional constant \textit{scalebroad}, related to the adaptive Gaussian broadening technique, was set to 0.2 in all the ShengBTE calculations, together with with 19\times19\times19, 19\times19\times19, and 15\times15\times12 q-point grids for \(\alpha\)-CaF$_2$, \(\delta\)-CaF$_2$, and \(\gamma\)-CaF$_2$, respectively.

C. Phonons

The second order interatomic force constants were calculated by the finite difference approach using the supercell method as implemented in the Phonopy package. Supercells of dimension 4 \times 4 \times 4, 2 \times 3 \times 2, and 2 \times 2 \times 4 were used for \(\alpha\)-CaF$_2$, \(\gamma\)-CaF$_2$, and \(\delta\)-CaF$_2$, respectively, leading to cells consisting of 192, 144, and 144 atoms. A finite difference step size of 0.01 Å was applied to displace the atoms. A q-point mesh of 50 \times 50 \times 50 was used for the BZ integration.

D. BTE thermal transport

The thermal transport calculations were carried out by taking into account anharmonic three-phonon interactions. Third-order force constants were computed from finite differences using the supercell method with the same sizes used in the calculations of the second-order force constants. Atomic displacements were created using the \texttt{thirdorder.py} script included in the ShengBTE distribution taking into account up to the 5th-nearest neighbors to truncate the three-body interactions, which gives well converged values of \(\kappa\). The thermal conductivity in the BTE is given by

\[
\kappa = \frac{1}{3V N_q} \sum_{q\gamma} C_{q\gamma} \gamma^2 \tau_{q\gamma}
\]

(1)

where \(V\) is the volume of the cell containing \(N\) atoms, \(q\) refers to the wave vector in the first Brillouin zone, \(N_q\) is the number of discrete q-points, \(\gamma\) is the mode index that refers to different phonon branches, \(C_{q\gamma}\) denotes the mode specific heat capacity at constant volume, \(\nu\) is the phonon group velocity (\(\nu_{q\gamma} = \nabla_{q\gamma} \omega_{q\gamma}\)), \(\tau\) is the phonon life time, which is related to the MFP \(\lambda = \nu \cdot \tau\).

The detailed effects of the cutoff-distance on the thermal conductivities are shown in section S3 of the supporting information. The second- and third-order interatomic force constants were fed into the ShengBTE package to calculate \(\kappa\) by iteratively solving the linearized phonon Boltzmann transport equation for temperatures ranging from 100 K to 900 K. Both isotropic and three-phonon scattering were considered. The isotropic scattering rates were calculated by applying the Pearson deviation coefficients incorporated in ShengBTE. The so-called proportional constant \textit{scalebroad}, related to the adaptive Gaussian broadening technique, was set to 0.2 in all the ShengBTE calculations, together with with 19\times19\times19, 19\times19\times19, and 15\times15\times12 q-point grids for \(\alpha\)-CaF$_2$, \(\delta\)-CaF$_2$, and \(\gamma\)-CaF$_2$, respectively.

E. Cahill-Pohl model

We estimate the amorphous limit of the thermal conductivity \(\kappa_{\text{CP}}\) using the Cahill-Pohl model, which is an extension of the Einstein model. While Einstein assumed that the thermal energy is transported between neighboring atoms vibrating with a single frequency, the Cahill-Pohl model proposes that the energy is transferred between collective vibrations. Therefore, the model includes a range of frequencies, instead of a single frequency used by Einstein. In this model, the thermal conductivity is expressed as follows (details in Ref.):

\[
\kappa_{\text{CP}} = \left(\frac{\pi}{6}\right)^{1/3} k_B n \frac{\pi}{\alpha^{3/2}} \sum_{\gamma} v_{\gamma} \left(\frac{T}{\alpha^{3/2}}\right) \int_0^{\infty} \frac{x^2 e^x}{(e^x-1)^2} dx,
\]

\[
x = \frac{T_{\alpha}^D}{T},
\]

(2)

where \(n\) is the density of the atoms in the solid (m$^{-3}$), \(v_{\gamma}\) is the low-frequency speed of sound (from acoustic phonons) for polarization \(\alpha\), \(T_{\alpha}^D = \frac{1}{2}\frac{v_{\gamma}}{n(6n)^{1/3}}\) is the characteristic temperature equivalent to the Debye temperature for that polarization which corresponds to the activation of all phonons. \(x\) is the reduced phonon energy and the summation runs over the vibrational polarizations (one longitudinal and two transverse acoustic branches). The \(v_{\gamma}\) of each acoustic group velocity was determined using harmonic lattice dynamics from Sec. [11C]

III. RESULTS AND DISCUSSION

We start out by validating the quality and predictive power of our CENT potential with respect to DFT results based on the three relevant phases \(\alpha\)-CaF$_2$, \(\gamma\)-CaF$_2$, and \(\delta\)-CaF$_2$. The thermodynamic properties including the transition pressures are well reproduced by CENT. As shown in Fig. S1 of the supplementary materials, the phase transition from \(\alpha\)-CaF$_2$ to \(\gamma\)-CaF$_2$ occurs at 8 GPa.
which is close to experimental measurements. Also, the enthalpy differences of the δ-CaF₂ and γ-CaF₂ decreases with increasing pressure. In fact, these two high pressure phases are energetically very close to each other, i.e., dropping from 12.7 to 2.1 meV/atom in the pressure range between 2 and 30 GPa. We then compare the dynamical properties predicted by the CENT potential with DFT values at 2 GPa. The phonons arising from the CENT potential as well as the phonon DOS agree well with the results from DFT (see Fig. S2 in the supplementary materials). Similarly, the lattice thermal conductivities from CENT are in excellent agreement with the DFT predictions, as shown in Fig. S3 in the supplementary material.

Next, we study the evolution of the thermal conductivity of the three phases as a function of pressure. Since the δ-CaF₂ phase exhibits imaginary phonon modes at 0 GPa, we focus on the pressure regime between 2 and 30 GPa within which all structures are dynamically stable. Fig. 1 plots the components of the thermal conductivity at selected temperatures, and shows that their values increase almost linearly with pressure. This increase in thermal conductivity can be rationalized in a first approximation by the decrease in volume $V$ in the denominator in Eq. (1) as the pressure increases. The room-temperature thermal conductivity of all three phases at different pressures and room temperature are also summarized in Table I.

![Graph showing thermal conductivity components](image)

**FIG. 1.** (color online) The components of the lattice thermal conductivities $\kappa_{x,y,z}$ of α-CaF₂ (panels (a) to (c)), γ-CaF₂ (panels (d) to (f)), and δ-CaF₂ (panels (g) to (i)), as a function of pressure at temperatures of 300, 600, and 900 K. DFT data are shown with blue crosses, while CENT results are shown with yellow squares (300 K), orange circles (600 K), and pink dots (900 K).

At all pressures, α-CaF₂ has a significantly higher value of $\kappa$ than any of the other two phases at a given temperature. Table I also contains the room-temperature zero-pressure value of the thermal conductivity, $\kappa_{\text{ambient}}$, of α-CaF₂ from other theoretical studies in the literature. We obtain $\kappa_{\text{ambient}} = 7.5 \, \text{Wm}^{-1}\text{K}^{-1}$, which is close to the value of 7.0 \ Wm$^{-1}$K$^{-1}$ reported by Plata et al. In comparison with experimental results from Andersson et al, our value of $\kappa_{\text{ambient}}$ is about 2.2 \ Wm$^{-1}$K$^{-1}$ lower than the experimental measurement of 9.7 \ Wm$^{-1}$K$^{-1}$ through a two-strip method.

Our values of $\kappa$ for δ-CaF₂ and γ-CaF₂ show that, unlike α-CaF₂, these two phases exhibit slight anisotropies along their three components. At 300 K, the components of $\kappa_{x,y,z}$ for the γ-CaF₂ and δ-CaF₂ phases at 2 GPa are approximately $\{2.1, 1.7, 1.6\}$ and $\{0.8, 0.8, 1.2\}$ Wm$^{-1}$K$^{-1}$, respectively, while $\kappa$ itself are 1.8 and 0.93 Wm$^{-1}$K$^{-1}$ for γ-CaF₂ and δ-CaF₂, respectively. The very low thermal conductivity of the δ-phase at low pressures can be primarily attributed to the soft acoustic phonon mode along K-Γ in the first Brillouin zone.

There are several factors leading to the decreased $\kappa$ of γ-CaF₂ and δ-CaF₂ compared to the cubic structure. Eq. (1) contains the product of heat capacity, phonon group velocity, and phonon mean free path, the effects of which we can study individually. We first investigate the heat capacities per unit volume at selected pressure and temperatures, and show its evolution in Fig. S4 of the SI. The heat capacity rapidly increases with temperature $T$, and is proportional to $T^3$ at low $T$, whereas it tends to a constant value at a high temperature, following the Dulong-Petit law. In the case of α-CaF₂, the obtained value of $C_v$ at zero pressure and at temperature 300 K is 65.57 J/m/K, which is comparable with the experimental value of 67.11 J/m/K. The obtained values of $C_v$ at temperature 300 K and pressure 2 GPa for α-CaF₂, δ-CaF₂, and γ-CaF₂ are 64.92, 65.10, and 64.64 J/m/K, respectively. The value of $C_v$ decreases with increasing pressure (see insets in Fig. S4 of the SI) at given temperature, and at 30 GPa reaches 58.29, 59.77, and 59.54 J/m/K for α-CaF₂, δ-CaF₂, and γ-CaF₂, respectively. Overall, the difference in $C_v$ among the three phases is minute (within less than 3 %) and cannot account for the strong deviations of $\kappa$.

We now turn our attention to the group velocities $v_g$ of the acoustic phonon modes, which are in general responsible for a large fraction of the thermal transport. Fig. 2 shows $v_g$ of the longitudinal and transverse acoustic (LA and TA) branches of γ-CaF₂ and δ-CaF₂, plotted on top of the values of α-CaF₂. Note that the δ-phase exhibits a particularly soft acoustic branch with a low $v_g$ along K-Γ (see Fig. S5 in the SI). Overall, α-CaF₂ has larger group velocities than either γ-CaF₂ or δ-CaF₂. To quantify the difference in the group velocities, we consider the mean values of the LA and the two TA modes, $\overline{v}_{g,LA}$, $\overline{v}_{g,TA_1}$, and $\overline{v}_{g,TA_2}$. The ratios of these average velocities of α-CaF₂ with respect to the γ and δ phases is $\{\overline{v}_{g,LA}, \overline{v}_{g,TA_1}, \overline{v}_{g,TA_2}\}_\alpha/\{\overline{v}_{g,LA}, \overline{v}_{g,TA_1}, \overline{v}_{g,TA_2}\}_\gamma = \{1.7, 1.7, 1.9\}$, and $\{\overline{v}_{g,LA}, \overline{v}_{g,TA_1}, \overline{v}_{g,TA_2}\}_\alpha/\{\overline{v}_{g,LA}, \overline{v}_{g,TA_1}, \overline{v}_{g,TA_2}\}_\delta = \{1.4, 1.5, 1.3\}$.


TABLE I. The components of the lattice thermal conductivity $\kappa_{x,y,z}$ using CENT in units of $Wm^{-1}K^{-1}$ at 300 K and at selected pressures, together with available values from the literature. Results from DFT calculations are given in parenthesis.

| Phase     | Components of $\kappa$ | 0 GPa          | 2 GPa          | 10 GPa         | 20 GPa         | 30 GPa         |
|-----------|------------------------|----------------|----------------|----------------|----------------|----------------|
| $\alpha$-CaF$_2$ | $\kappa_x = \kappa_y = \kappa_z$ | 7.5            | 9.4 (9.2)      | 17.6 (18.8)    | 27.1           | 37.5 (38.2)    |
| $\delta$-CaF$_2$ | $\kappa_x = \kappa_y$ | 0.9 (0.9)      | 2.3 (2.9)      | 4.6            | 7.2 (10.0)     |                |
| $\gamma$-CaF$_2$ | $\kappa_x$ = 1.8      | 2.1 (2.3)      | 3.5 (4.1)      | 5.9            | 8.4 (12.3)     |                |
| $\gamma$-CaF$_2$ | $\kappa_z$ = 1.6      | 1.7 (2.3)      | 3.2 (4.8)      | 5.7            | 7.9 (10.8)     |                |

Hence, the group velocities of $\alpha$-CaF$_2$ is almost twice as high as the corresponding values in $\gamma$-CaF$_2$ and $\delta$-CaF$_2$.

Further, the contributions of acoustic modes to the thermal transport is influenced by their interaction with the optical modes, i.e., the amount of heat that is scattered through optical phonons. In general, phases with larger, complex structures tend to have larger contributions from optical scattering, with stronger coupling between acoustic and optical modes. Fig. 2 shows the fraction of acoustic modes contributing to the total thermal conductivity, $r_\kappa = \kappa_{\text{acoustic}}/\kappa_{\text{total}}$ for the $\alpha$, $\gamma$, and $\delta$ phase. At any pressure and temperature, $\alpha$-CaF$_2$ exhibits the largest value of $r_\kappa$. Both $\gamma$-CaF$_2$ and $\delta$-CaF$_2$ show strong contributions of optical phonon scattering, in particular for $\delta$-CaF$_2$ at low lower pressures. Again, this behavior can be attributed to the soft-mode in one of the acoustic branches of $\delta$-CaF$_2$ at 2 GPa, which becomes less pronounced with increasing pressure as shown in Fig. S5 in the SI.

We also compare the phonon MFP in Fig. 4 at 2 and 30 GPa at a temperature of 300 K. Overall, the MFPs of the $\alpha$-phase are longer than either of the high-pressure phases. In fact, the MFP of a significant fraction of modes are shorter than the average inter-atomic distance of $\approx 2.4$ Å in both the $\gamma$ and $\delta$-phases, leading to an inaccurate description of thermal transport within the BTE by dramatically underestimating the value of $\kappa_{\text{CP}}$.

To address this issue, we assess the limitations of the BTE by comparing its results to the Cahill-Pohl model, which provides an estimate of the lower bound in the amorphous limit, $\kappa_{\text{CP}}$. Fig. 5 shows the values of $\kappa_{\text{CP}}$ as a function of temperature and pressures for the $\alpha$, $\gamma$, and $\delta$-CaF$_2$. We observe two very clear trends: (a) $\kappa_{\text{CP}}$ increases with temperature at a given pressure, plateauing out above $\approx 600$ K (see top row in Fig. 5), and (b) $\kappa_{\text{CP}}$ increases steadily with pressure at constant temperature (see bottom row in Fig. 5). The values of $\kappa_{\text{CP}}$ are particularly high for $\delta$-CaF$_2$, which indicates that an especially large error can be expected in the BTE model.

To assess the limits of the BTE, we map out the boundary in $T$ and $p$ where $\kappa_{\text{BTE}}$ drops below the amorphous limit, $\kappa_{\text{CP}}$. Fig. 6 plots the $\kappa_{\text{BTE}}$ and $\kappa_{\text{CP}}$ at selected temperatures as a function of pressure. For $\alpha$-CaF$_2$, the thermal conductivities predicted through the BTE are reliable, as their values remain above $\kappa_{\text{CP}}$ for all pressures and temperatures considered here. However, the BTE
FIG. 4. (color online) Phonon mean free path (MFP) of all phonon modes as a function of frequency at pressures of 2 GPa (first row) and 30 GPa (second row) of α-CaF$_2$ (panels (a) and (b)), γ-CaF$_2$ (panels (c) and (d)), and δ-CaF$_2$ (panels (e) and (f)).

FIG. 5. (color online) The amorphous limit of the thermal conductivity $\kappa$ as a function of pressure for $\alpha$-CaF$_2$ (a) and (b), $\gamma$-CaF$_2$ (c) and (d), and $\delta$-CaF$_2$ (e) and (f). Cahill-Pohl model (green triangles) at 300 and 900 K together with the results of BTE (red circles) at the same conditions. The values obtained from DFT results are shown with blue symbols. The calculated transition boundary where the $\kappa_{CP}/\kappa_{BTE}$ for $\gamma$-CaF$_2$ and $\delta$-CaF$_2$ are shown in panel (g), where the shaded regions indicate the $T - p$-range where BTE is reliable.

FIG. 6. (color online) The thermal conductivity $\kappa$ as a function of pressure for $\alpha$-CaF$_2$ (a) and (b), $\gamma$-CaF$_2$ (c) and (d), and $\delta$-CaF$_2$ (e) and (f) Cahill-Pohl model (green triangles) at 300 and 900 K together with the results of BTE (red circles) at the same conditions. The values obtained from DFT results are shown with blue symbols. The calculated transition boundary where the $\kappa_{CP}/\kappa_{BTE}$ for $\gamma$-CaF$_2$ and $\delta$-CaF$_2$ are shown in panel (g), where the shaded regions indicate the $T - p$-range where BTE is reliable.

breaks down for $\delta$-CaF$_2$ and $\gamma$-CaF$_2$, especially at low temperatures and low pressures. The transition boundary where $\kappa_{BTE}$ crosses $\kappa_{CP}$ in $T$ and $p$ is mapped out in Fig. 5(g), showing that BTE only yields reliable results within the regime of high pressure and low temperatures.

IV. CONCLUSIONS

In summary, we studied the effect of pressure and temperatures on the thermal transport properties of three crystalline CaF$_2$ phases, using DFT and a machine-learning based interatomic potential. Our results show that the two high-pressure phases, $\delta$-CaF$_2$ and $\gamma$-CaF$_2$, exhibit significantly lower thermal conductivities $\kappa$ than the cubic $\alpha$-phase. We argue that the source of this large difference in $\kappa$ stems from lower group velocities of the acoustic modes, and the larger contributions of phonon scattering events involving the optical modes in the $\delta$ and $\gamma$-phase which additionally impedes the transport of heat. A careful analysis of the phonon scattering shows that the MFPs (and the associated phonon lifetimes) are extremely short for the $\delta$ and $\gamma$-phases, lead-
ing to the low values of $\kappa$. In fact, for high temperatures and at low pressures the MFPs are so short that they drop below the mean atomic bond lengths, and we expect that the thermal conductivity will eventually converge to the amorphous limit which we estimate using the Cahill-Pohl model. Despite these limitations, our results show that the high-pressure phases exhibit around a factor of 5 times lower thermal conductivity than the ambient ground state.

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1 W. Liang, V. Ilchenko, D. Eliyahu, A. Savchenkov, A. Matsko, D. Seidel, and L. Maleki, Nature communications 6 (2015).
2 C. Cazorla and D. Errandonea, Physical review letters 113, 235902 (2014).
3 A. Lyberis, A. J. Stevenson, A. Suganuma, S. Ricaud, F. Druon, F. Herbst, D. Vivien, P. Gredin, and M. Mortier, Optical Materials 34, 965 (2012).
4 L. Sang, M. Liao, Y. Koide, and M. Sumiya, Applied Physics Letters 98, 3502 (2011).
5 V. Liberman, T. Bloomstein, M. Rothschild, J. Sedlacek, R. Uttaro, A. Bates, C. Van Peski, and K. Orvek, Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures Processing, Measurement, and Phenomena 17, 3273 (1999).
6 M. Daimon and A. Masumura, Applied optics 41, 5275 (2002).
7 C. Wagner and N. Harned, Nature Photonics 4, 24 (2010).
8 W. Liang, V. Ilchenko, D. Eliyahu, A. Savchenkov, A. Matsko, D. Seidel, and L. Maleki, Nature communications 6, 7371 (2015).
9 X. C. Luo, J. N. Sun, W. L. Chang, and J. M. Ritchie, in Key Engineering Materials, Vol. 516 (Trans Tech Publ, 2012) pp. 408–413.
10 L. Sang, M. Liao, Y. Koide, and M. Sumiya, Applied Physics Letters 98, 103502 (2011).
11 K. F. Seifert and B. Bunsenges, Phys. Chem. 70, 1041 (1966).
12 D. P. Dandekar and J. C. Jamieson, Trans. Am. Crystallogr. Assoc. 5, 19 (1969).
13 L. Gerward, J. S. Olsen, S. Steenstrup, M. Malinowski, S. Åsbirk, and A. Waskowska, Journal of applied crystallography 25, 578 (1992).
14 S. Dorfman, F. Jiang, Z. Mao, A. Kubo, V. Prakapenka, and T. Duffy, in AGU Fall Meeting Abstracts, Vol. 1 (2007) p. 1522.
15 S. Speziale and T. S. Duffy, Phys. Chem. Miner 29, 465 (2002).
16 J. H. Burnett, Z. H. Levine, and E. L. Shirley, Phys. Rev. B 64, 241102(R) (2001).
17 X. Wu, S. Qin, and Z. Y. Wu, Phys. Rev. B 73, 134103 (2006).
18 H. Shi, W. Luo, B. Johansson, , and R. Ahujia, J. Phys. Condens态 Matter 21, 415501 (2009).
19 F. S. Elkin, O. B. Tsiok, L. G. Khvostantsev, , and V. V. Brazhkin, J. Exp. Theor. Phys. 100, 971 (2005).
20 S. M. Dorfman, F. Jiang, Z. Mao, A. Kubo, Y. Meng, V. B. Prakapenka, and T. S. Duffy, Physical Review B 81, 174121 (2010).
21 J. R. Nelson, R. J. Needs, and C. J. Pickard, Physical Review B 95, 054118 (2017).
22 F. Charvat and W. Kingery, Journal of the american ceramic society 40, 306 (1957).
23 K. A. McCarthy and S. S. Ballard, Journal of Applied Physics 31, 1410 (1960).
24 G. A. Slack, Phys. Rev. 122, 1451 (1961).
25 P. Lindan and M. Gillan, Journal of Physics: Condensed Matter 3, 3929 (1991).
26 Y.-Y. Qi, T. Zhang, Y. Cheng, X.-R. Chen, D.-Q. Wei, and L.-C. Cai, Journal of Applied Physics 119, 095103 (2016).
27 S. Andersson and G. Backstrom, Journal of Physics C: Solid State Physics 20, 5951 (1987).
28 S. A. Ghasemi, A. Hofstetter, S. Saha, and S. Goedecker, Physical Review B 92, 045131 (2015).
29 S. Faraji, S. A. Ghasemi, S. Rostami, R. Rasoulkhani, B. Schaefer, S. Goedecker, and M. Amsler, Physical Review B 95, 104105 (2017).
30 M. Amsler, S. Rostami, H. Tahmasbi, E. Rahmatizad, S. Faraji, R. Rasoulkhani, and S. A. Ghasemi, Computer Physics Communications , 107415 (2020).
31 H. A. Eivari, S. A. Ghasemi, H. Tahmasbi, S. Rostami, S. Faraji, R. Rasoulkhani, S. Goedecker, and M. Amsler, Chem. Mater. 29, 8594 (2017).
32 R. Rasoulkhani, H. Tahmasbi, S. A. Ghasemi, S. Faraji, S. Rostami, and M. Amsler, Phys. Rev. B 96, 064108 (2017).
33 S. Faraji, S. A. Ghasemi, B. Parsaeifard, and S. Goedecker, Physical Chemistry Chemical Physics (2019).
34 P. Giannozzi, S. Baroni, N. Bonini, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, G. L. Chiarotti, M. Cococcioni, I. Dabo, A. Dal Corso, S. de Gironcoli, S. Fabris, G. Fratesi, R. Gebauer, U. Gerstmann, C. Gougoussis, A. Kokalj, M. Lazzi, L. Martin-Samos, N. Marzari, F. Mauri, R. Mazzarello, S. Paolini, A. Pasquarello, L. Paulatto, C. Sbraccia, S. Scandolo, G. Scuflaro, A. P. Seitsonen, A. Smogunov, P. Umari, and R. M. Wentzcovitch, Journal of Physics: Condensed Matter 21, 395502 (19pp) (2009).
35 P. Giannozzi, O. Andreussi, T. Brumme, O. Bubau, M. B. Nardelli, M. Calandra, R. Car, C. Cavazzoni, D. Ceresoli, M. Cococcioni, N. Colonna, I. Carmimeo, A. D. Corso, S. de Gironcoli, P. delugas, R. A. D. Jr, A. Ferretti, A. Floris, G. Fratesi, G. Fugallo, R. Gebauer, U. Gerstmann, F. Giustino, T. Gorni, J. Jia, M. Kawamura, H.-Y. Ko, A. Kokalj, E. Küçükbir, M. Lazzi, M. Marsili, N. Marzari, F. Mauri, N. L. Nguyen, H.-V. Nguyen, A. O. de-la Roza, L. Paulatto, S. Poncé, D. Rocca, R. Sabatini, B. Santra, M. Schlipf, A. P. Seitsonen, A. Smogunov, I. Timrov, T. Thou-
36 Hauser, P. Umari, N. Vast, X. Wu, and S. Baroni, Journal of Physics: Condensed Matter 29, 465901 (2017).
37 J. P. Perdew, K. Burke, and M. Ernzerhof, Physical review letters 77, 3865 (1996).
38 H. J. Monkhorst and J. D. Pack, Phys. Rev. B 13, 5188 (1976).
39 D. Vanderbilt, Phys. Rev. B 41, 7892 (1990).
40 A. Togo and I. Tanaka, Scripta Materialia 108, 1 (2015).
41 W. Li, J. Carrete, N. A. Katcho, and N. Mingo, Computer Physics Communications 185, 1747 (2014).
42 T. Luo, J. Garg, J. Shiomi, K. Esfarjani, and G. Chen, EPL (Europhysics Letters) 101, 16001 (2013).
43 D. G. Cahill and R. O. Pohl, Annual review of physical chemistry 39, 93 (1988).
44 M. Kaviany, Heat transfer physics (Cambridge University Press, 2014).
45 J. J. Plata, P. Nath, D. Usanmaz, J. Carrete, C. Toher, M. de Jong, M. Asta, M. Fornari, M. B. Nardelli, and S. Curtarolo, npj Computational Materials 3, 45 (2017).
46 Y.-Y. Qi, T. Zhang, Y. Cheng, X.-R. Chen, D.-Q. Wei, and L.-C. Cai, Journal of Applied Physics 119, 095103 (2016).
47 P. B. Allen and J. L. Feldman, Physical Review B 48, 12581 (1993).