High intrinsic lattice thermal conductivity in monolayer MoSi$_2$N$_4$

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Abstract

Very recently, a novel two-dimension (2D) MXene, MoSi$_2$N$_4$, was successfully synthesized with excellent ambient stability, high carrier mobility, and moderate band gap (2020 Science 369 670). In this work, the intrinsic lattice thermal conductivity of monolayer MoSi$_2$N$_4$ is predicted by solving the phonon Boltzmann transport equation based on the first-principles calculations. Despite the heavy atomic mass of Mo and complex crystal structure, the monolayer MoSi$_2$N$_4$ unexpectedly exhibits a quite high lattice thermal conductivity over a wide temperature range between 300 to 800 K. At 300 K, its in-plane lattice thermal conductivity is 224 Wm$^{-1}$K$^{-1}$. The detailed analysis indicates that the large group velocities and small anharmonicity are the main reasons for its high lattice thermal conductivity. We also calculate the lattice thermal conductivity of monolayer WSi$_2$N$_4$, which is only a little smaller than that of MoSi$_2$N$_4$. Our findings suggest that monolayer MoSi$_2$N$_4$ and WSi$_2$N$_4$ are potential 2D materials for thermal transport in future nano-electronic devices.

1. Introduction

Since the successful exfoliation of monolayer graphene [1], there have been extensive efforts to find novel two-dimensional (2D) materials due to their unusual mechanical, thermal, optoelectric, piezoelectric, and thermoelectrical properties [2–10]. Owing to these unique properties, 2D materials have become promising candidates for optoelectronics [11], field-effect transistors [12], and energy applications [13, 14]. Many classes of monolayer 2D materials have been fabricated, such as transition metal dichalcogenides [2, 15], h-BN [16], phosphorene [17], borophene [18], and silicene [19]. It may have difficulties if these monolayer materials are directly applied in integrated nanoelectronic devices because of their restricted properties. For example, graphene and borophene have no band gap [20, 21] while monolayer BN has an excessively wide band gap [22]. Monolayer phosphorene and silicene are unstable upon exposure [19, 23]. The carrier mobility in monolayer MoS$_2$ is quite low [24]. Thus, the discovery of a desirable monolayer 2D material with a moderate band gap and high carrier mobility remains a primary research goal in materials science and physics.

Recently, a high-quality 2D MXene, MoSi$_2$N$_4$, was successfully synthesized with excellent ambient stability, moderate band gap, and considerable carrier mobility [25]. Experimental results [25] demonstrated that MoSi$_2$N$_4$ has a band gap of about 1.94 eV. Furthermore, large hole and electron mobilities of monolayer MoSi$_2$N$_4$ are predicted to be about 1200 and 270 cm$^2$V$^{-1}$s$^{-1}$ [25], which are four to six times higher than those of MoS$_2$ monolayer [26]. Since the synthesis of MoSi$_2$N$_4$, intensive research
efforts have been devoted to unearthing its novel properties [27–35]. First principles calculations revealed that the large thermopower of monolayer MoSi₂N₄ can be obtained in a range of chemical potential from 0 to 1 eV [27]. Cao et al [28] investigated the electrical contact of monolayer MoSi₂N₄ and an ultralow Schottky barrier height was observed in MoSi₂N₄/NbS₂ contact [28], which is beneficial for the nano-electronic device applications. The theoretical calculations demonstrated that the piezoelectricity MoSi₂N₄ enables actuating new electronic components of nanoscale devices [32].

Thermal transport is an important property for materials in many applications including thermal barrier coating [36], heat management [37], and thermoelectric energy conversion [38]. Especially the phonon transport is an essential part of designing all power-dissipating devices [39, 40]. 2D materials are ideal platforms to investigate fundamental carrier transport and provide new directions for thermal management and energy control. Phonon transport phenomena are related to various intriguing applications based on 2D materials [37]. In recent years, the lattice thermal conductivities of 2D materials have attracted considerable interest [41–53]. For these reasons, the study of the thermal transport property of monolayer MoSi₂N₄ is urgently called to speed up its application.

In this paper, we have systematically investigated the intrinsic thermal transport properties of monolayer MoSi₂N₄ by iteratively solving the Boltzmann transport equation. It is found that MoSi₂N₄ unexpectedly exhibits a quite high and almost isotropic lattice thermal conductivity despite its great average atomic mass and complex crystal structure. To further explain the mechanism of the high thermal conductivities, we also discuss the phonon lifetimes, group velocities, and Grüneisen parameters of the monolayer MoSi₂N₄.

2. Theoretical methods

The crystal structure of monolayer MoSi₂N₄ is fully optimized by the Vienna \textit{ab initio} simulation package [54, 55] based on the density functional theory. The projected augmented wave method [56, 57] and generalized gradient approximation with the Perdew–Burke–Ernzerh of exchange–correlation functional [58] are used. The plane-wave cutoff energy of 520 eV is used with a 12 \times 12 \times 1 k-mesh. Both the lattice constants and internal atomic positions are allowed to relax until the maximal residual Hellmann–Feynman forces are less than 0.0001 eV Å⁻¹. To avoid interactions with other neighboring layers, a vacuum space of 15 Å is taken.

After optimizing the crystal structure, we further perform the calculations of the second- and third-order interatomic force constants (IFCs) with the finite displacement method. The second-order IFCs in the harmonic approximation and the phonon dispersions of monolayer MoSi₂N₄ are calculated by using the PHONOPY code [59]. And the third-order IFCs and their lattice thermal conductivities are obtained based on the PHONOPY code [60], which solves the phonon Boltzmann transport equation by using the iterative self-consistent algorithm. The lattice thermal conductivity is defined as [60]:

$$\kappa = \frac{1}{NV} \sum_\lambda C_\lambda v_\lambda \otimes v_\lambda \tau_\lambda, \tag{1}$$

where $N$ and $V$ are the number of unit cells in the crystal, the volume of a unit cell. $v_\lambda$ and $\tau_\lambda$ are the group velocity and lifetime of the phonon mode $\lambda$, respectively. The method has already been widely used in the prediction of thermal conductivities for 2D materials [42, 44, 45, 52–54]. The energy convergence criteria for monolayer MoSi₂N₄ is 10⁻⁷ eV. A $4 \times 4 \times 1$ supercell (112 atoms) with a $3 \times 3 \times 1$ k-mesh is used to calculate the second- and third-order IFCs. The lattice thermal conductivity of monolayer MoSi₂N₄ is calculated with a cutoff distance of 5.0 Å and a q-mesh of $30 \times 30 \times 1$. The phase space for three-phonon processes P3 is also calculated by the ShengBTE code [61].

3. Results and discussion

3.1. Crystal structure and phonon dispersions

The structure of monolayer MoSi₂N₄ has seven atoms per unit cell. As shown in figure 1, the crystal exhibits a sandwiched structure, where the 2H MoS₂-type MoN₂ layer is sandwiched between two slightly buckled SiN layers. Monolayer MoSi₂N₄ holds a mirror paralleling to the horizontal plane, inversion asymmetry, and C₃ rotation symmetry. The lattice constants obtained in our calculations are $a = b = 2.911$ Å, which are a little smaller than those of monolayer MoS₂ (3.16 Å) [9]. The distances between Si and its adjacent N (N1 and N2) are 1.748 and 1.755 Å, respectively. The distance of Mo–Si is 2.093 Å. The thicknesses ($d_{ij}$) of the vertical MoSi₂N₄ plane is 7.00 Å. These results are in good agreement with the previous reports [25, 27]. We also check the electronic properties by calculating its electronic band structure and partial density of states (PDOS), which is given in figure S1 (https://stacks.iop.org/NJP/23/033005/mmedia). It is found that
monolayer MoSi$_2$N$_4$ exhibits an indirect band gap of 1.77 eV with the valence band maximum (VBM) and conduction band minimum (CBM) located at $\Gamma$ and $K$ points, respectively, which is also consistent with the previous studies [25, 27, 29, 30]. The band gap could be improved to be 2.30 eV based on the Heyd, Scuseria, Ernzerhof (HSE) functional calculations [25]. The wide band gap implies that the lattice thermal conductivity is dominant in the total thermal conductivity of monolayer MoSi$_2$N$_4$. It can be seen from the PDOSs in figure S1 that the VBM and CBM are mostly dominated by Mo’s d orbitals, with a small contribution from N’s p states. There is a strong hybridization between Mo’s d (Si’s p) and N’s p orbitals from about $-10.0$ to $-2.0$ eV and 2.0 to 6.0 eV. The result is consistent with the charge analysis, indicating about 2.2 e (1.5 e) transferring from Si (Mo) atom to its adjacent N atom, respectively [27]. The strong hybridization and large charge transfer suggest that there are strong interactions between Mo (Si) and N atoms.

The phonon dispersions play a significant role in the precise calculation of phonon transport properties.

![Figure 1.](image1.png)

**Figure 1.** (a) Top and (b) side views of the crystal structure of monolayer MoSi$_2$N$_4$. The primitive unit cell is indicated by a black hexagonal in (a). The red, blue, and brown balls represent Mo, Si, and N atoms, respectively.

![Figure 2.](image2.png)

**Figure 2.** (a) Phonon dispersions and (b) DOS of monolayer MoSi$_2$N$_4$. The average sound velocity can be determined by the formula $v_{\text{avg}} = \frac{1}{3} v_{\text{LA}} + \frac{1}{3} v_{\text{TA}} + \frac{1}{3} v_{\text{ZA}}$, where $v_i$ represents the x or y axis. Along the x axis, the sound velocities in the long-wavelength limit are 10.7, 6.1, and 2.0 km s$^{-1}$ for the LA (in-plane longitudinal acoustic), TA (in-plane transverse acoustic), and ZA (out-of-plane transverse acoustic) phonons respectively. These values are higher than...
Table 1. Calculated sound velocities of monolayer MoSi$_2$N$_4$ along $x$ and $y$ axes in the unit of km s$^{-1}$.

|          | LA   | TA   | ZA   | Average |
|----------|------|------|------|---------|
| $x$ axis | 10.7 | 6.1  | 2.0  | 2.9     |
| $y$ axis | 10.8 | 6.1  | 2.2  | 3.1     |

Figure 3. Calculated in-plane lattice thermal conductivity ($\kappa_{xx}$) of monolayer MoSi$_2$N$_4$ from 300 to 800 K.

those of silicene (8.8, 5.4, and 0.63 km s$^{-1}$ for the LA, TA, and ZA phonons) [62] and MoS$_2$ (6.6 and 4.3 for the LA and TA phonons) [62] but much smaller than those of graphene (19.9 and 12.9 km s$^{-1}$ for the LA and TA phonons) [63]. The sound velocities of monolayer MoSi$_2$N$_4$ along the $y$ axis are almost identical to that in the $x$ axis. The large sound velocities are one of the main reasons for the high lattice thermal conductivities of monolayer MoSi$_2$N$_4$ as we will show later.

3.2. Lattice thermal conductivity

We then calculate the temperature-dependent lattice thermal conductivity ($\kappa_{xx}$) of monolayer MoSi$_2$N$_4$, as depicted in figure 3. It is noted that the in-plane thermal conductivity $\kappa_{yy}$ is equal to $\kappa_{xx}$ due to its hexagonal structure. The intrinsic lattice thermal conductivity decreases with the increase of temperature, which could be explained by the Umklapp scatterings of phonons [64]. At 300 K, the lattice thermal conductivities of MoSi$_2$N$_4$ are 224 W m$^{-1}$ K$^{-1}$, which is much higher than those of the other well-known 2D semiconductors, such as black phosphorene (30.15 W m$^{-1}$ K$^{-1}$ (zigzag), 13.65 W m$^{-1}$ K$^{-1}$ (armchair)) [50], monolayer 2H-MoTe$_2$ (42.2 W m$^{-1}$ K$^{-1}$) [51], MoS$_2$ (83 W m$^{-1}$ K$^{-1}$ [52] or 23.2 W m$^{-1}$ K$^{-1}$ [65]) and blue phosphorene (106.6 W m$^{-1}$ K$^{-1}$) [53], while much lower than that of monolayer hexagonal BN, BP, BAs [66], C$_3$N [67], and graphene [68] with low average atomic mass. It is noted that the thermal conductivity of MoSi$_2$N$_4$ is even much higher than those of widely used electronic materials such as Si (142 W m$^{-1}$ K$^{-1}$) [69]. Hence, the satisfactory lattice thermal conductivity of MoSi$_2$N$_4$ could guarantee heat removal in the corresponding nano-electronic devices.

To deeply understand the lattice thermal conductivity of monolayer MoSi$_2$N$_4$, we then further calculate the cumulative lattice thermal conductivity of MoSi$_2$N$_4$ at 300 K, given in figure 4(a). The cumulative lattice thermal conductivity first increases with the increase of mean free path (MFP), and then gradually saturates when the phonon MFP is equal to or larger than 1000 nm, which is much longer than those of black phosphorene (66/83 nm) [50], but shorter than graphene [68]. The phonon MFP in MoSi$_2$N$_4$ is much longer than those in the other 2D materials, leading to a much higher thermal conductivity. The representative MFP (rMFP) of materials is useful for studying the size effects on the diffusive or ballistic phonon transport. The rMFP means the phonons whose MFP is smaller than their rMFP contribute to half of the total lattice thermal conductivity. The rMFP of MoSi$_2$N$_4$ is 156.3 nm, and the values are about ten times that of phosphorene (17/15 nm [50]).

We also calculated the frequency-dependent lattice thermal conductivity of monolayer MoSi$_2$N$_4$ at 300 K, which is presented in figure 4(b). The width of each column in the figure is 2.0 THz. The summation of all columns represents the total thermal conductivity. It is found that the phonon below 15 THz contribute most of (96%) the lattice thermal conductivity in monolayer MoSi$_2$N$_4$. Furthermore, we also analyzed the contribution of acoustic and optical phonons. It is found that the acoustic phonons contribute about 55% and the optical ones contribute about 45% of the thermal conductivity in both directions. The
Figure 4. (a) Normalized directional cumulative lattice thermal conductivity ($K_{\text{L}}$) with respect to the phonon MFP and (b) frequency-dependent in-plane lattice thermal conductivity of monolayer MoSi$_2$N$_4$ at 300 K. In (b), the phonons above 20 THz contribute little to the thermal conductivity, which is not shown here.

Figure 5. (a) Square of the group velocities, (b) phonon lifetimes, and (c) frequency-dependent mode Grüneisen parameters of monolayer MoSi$_2$N$_4$ at 300 K.

large contribution of the optical phonons is due to the large number of low-frequency optical modes of the complex structure of monolayer MoSi$_2$N$_4$.

In addition, it should be noted that there is an inverse relationship between the lattice thermal conductivity of a material and its phase space for three-phonon scattering P3, which represents the relative number that satisfies the energy and momentum conservation selection rules [70]. Here, we have also calculated the phase space for three-phonon processes P3 for the monolayer MoSi$_2$N$_4$, which is 0.002 21. This value is comparatively lower than those in materials such as the monolayer GaN [71] and well-known semiconductor Si [70]. The low value of P3 also implies that the monolayer MoSi$_2$N$_4$ has high intrinsic lattice thermal conductivity.

3.3. Phonon group velocities, lifetimes, and Grüneisen parameters

To understand the underlying mechanism of the high intrinsic lattice thermal conductivity in MoSi$_2$N$_4$, we further analyze its phonon group velocities, lifetimes, and Grüneisen parameters. The squares of the phonon group velocities are plotted in figure 5(a). The large values of squares of the group velocities almost lie below about 15 THz which could reach more than 100 km$^2$ s$^{-2}$ which are much larger than those of monolayer MoS$_2$ [65]. Since the lattice thermal conductivity is proportional to the squares of group velocities, therefore the large group velocities in figure 5(a) as well as the large sound velocities in table 1 are the important reasons for its high thermal conductivity.

The frequency-dependent phonon lifetimes of MoSi$_2$N$_4$ are calculated by using the PHONO3PY code from the third-order anharmonic IFCs, as displayed in figure 5(b). The phonon lifetimes at the low frequency (acoustic phonon modes) are much longer than those of high-frequency optical modes. Most of the phonon lifetimes in MoSi$_2$N$_4$ are in the range from 0 to 50 ps. The lifetimes are larger than those of monolayer MoS$_2$ [65], and even higher than those of penta-graphene (PG) and hydrogenated PG (HPG), while the lattice thermal conductivities of PG (350 W m$^{-1}$ K$^{-1}$) [72] and HPG (616 W m$^{-1}$ K$^{-1}$) [72] are...
much larger than that of MoSi$_2$N$_4$. The results imply that the long phonon lifetimes contribute significantly to the large thermal conductivity of monolayer MoSi$_2$N$_4$. Finally, we give the mode-dependent Grüneisen parameters ($\gamma$) of monolayer MoSi$_2$N$_4$, which can provide crucial information on the anharmonic interactions of phonons. The larger $\gamma$ implies stronger anharmonicity, which leads to low lattice thermal conductivity. Figure 5(c) indicates that Grüneisen parameters of MoSi$_2$N$_4$ are dominantly located in the range from $-1.5$ to $1.5$. The range is smaller than those of PG, HPG, and graphene ($-8$ to $2$) [72] which have ultra-high lattice thermal conductivities. The long lifetimes and small Grüneisen parameters indicate the small anharmonicity in monolayer MoSi$_2$N$_4$, which is another important reason for its high lattice thermal conductivity. This weak anharmonicity is attributed to the strong Mo–N and Si–N atomic interactions since Young’s modulus of MoS$_2$N$_4$ (479 GPa) is much higher than that of MoS$_2$ (270 GPa) [25].

### 3.4. Comparative study with monolayer WSi$_2$N$_4$

Finally, we compare MoSi$_2$N$_4$ with another 2D MXene (WSi$_2$N$_4$), which has also been successfully synthesized in the recent experiment [25]. Compared with monolayer MoSi$_2$N$_4$, WSi$_2$N$_4$ has the same crystal structure and similar band characteristics [25], but a wider band gap [25] and higher atomic density. To understand the difference of phonon transport properties between WSi$_2$N$_4$ and MoSi$_2$N$_4$, we further calculate the lattice thermal conductivity of monolayer WSi$_2$N$_4$, as gathered in figure S2. Monolayer WSi$_2$N$_4$ also exhibits high lattice thermal conductivity. At 300 K, the lattice thermal conductivity is 219 W m$^{-1}$ K$^{-1}$. The thermal conductivities of monolayer MoSi$_2$N$_4$ and WSi$_2$N$_4$ are smaller than that of SiN$_4$ (371 W m$^{-1}$ K$^{-1}$ at 300 K [73]) with similar Si–N bonds. We notice that although the atomic mass of W is much larger than that of Mo, the lattice thermal conductivity of WSi$_2$N$_4$ is slightly lower than that of MoSi$_2$N$_4$. The similar thermal conductivity results from their similar phonon spectra, the square of the group velocities, phonon lifetimes, and Gruneisen parameter as shown in figure S3.

### 3.5. Discussion

In 1972, Slack investigated many nonmetallic crystals with high thermal conductivity (>100 W m$^{-1}$ K$^{-1}$ at 300 K) and found four characteristics of them: (1) low average atomic mass, (2) simple crystal structure, (3) strong interatomic bonding, and (4) low anharmonicity [74]. In our case, MoSi$_2$N$_4$ and WSi$_2$N$_4$ have quite complex crystal structures (seven atoms in a unit cell) and great average atomic masses. However, they unexpectedly exhibit quite high lattice thermal conductivities (>200 W m$^{-1}$ K$^{-1}$ at 300 K). We think that the high thermal conductivities of MoSi$_2$N$_4$ and WSi$_2$N$_4$ are possibly due to their particular sandwiched structure, in which the heavy W or Mo layer is the inner layer while the light Si–N layers are the outer layers. Theinner and outer layers are in parallel connection and therefore the heat could still transfer fast in the Si–N layers despite the heavy Mo or W layers. This is possibly also the reason why the MoSi$_2$N$_4$ and WSi$_2$N$_4$ exhibit almost the same size of lattice thermal conductivity.

### 4. Conclusions

We investigate the lattice thermal conductivities of monolayer MoSi$_2$N$_4$ based on first-principles calculations and the Boltzmann transport equation. Unexpectedly, we find that its intrinsic lattice thermal conductivity (224 W m$^{-1}$ K$^{-1}$ at 300 K) are much higher than those of the other well-known semiconductors, such as black phosphorene, blue phosphorene, monolayer 2H-MoTe$_2$, and MoS$_2$. The lattice thermal conductivities of monolayer MoSi$_2$N$_4$ are almost independent of direction due to its isotropic structure. The detailed analysis indicates that the large lattice thermal conductivity of MoSi$_2$N$_4$ is attributed to the high phonon group velocities, long phonon lifetimes, and small Grüneisen parameters compared to the other well-known 2D materials. Besides, we compare the lattice thermal conductivities of monolayer MoSi$_2$N$_4$ and WSi$_2$N$_4$. It is found that the lattice thermal conductivity of WSi$_2$N$_4$ is only a little lower than those of monolayer MoSi$_2$N$_4$. We think that the high thermal conductivities of MoSi$_2$N$_4$ and WSi$_2$N$_4$ is possible due to their particular sandwiched structure, in which the Si–N layers are mainly responsible for the heat transportation. The high lattice thermal conductivities of monolayer MoSi$_2$N$_4$ and WSi$_2$N$_4$ making them promising building blocks for heat dissipation in nanoelectronics and microelectronics.

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**Data availability statement**

All data that support the findings of this study are included within the article (and any supplementary files).

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