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ABSTRACT

It is conventionally believed that lattice thermal conductivity (κ) decreases with increasing atomic mass (negative atomic-mass correlation), and the high κ can only occur in crystals composed of strongly bonded light elements. By solving the fundamental thermal conductivity equation using first-principles calculations, here we reveal the anomalous κ departing from the long-held concept, that is, a positive atomic-mass correlation and high κ with heavy elements and weakly bonded interaction. We demonstrate this anomalous phenomenon by performing calculations of the cross-plane κ of the layered compounds, i.e., the h-BX family with X = N, P, and As. We find that the anomalous increase in the cross-plane κ with X going from N to As results in the cross-plane/in-plane conductivity ratio, generally expected to be much smaller than 1 in layered compounds, reaching as large as 2.6 at low temperatures. We also find that the unusually high cross-plane κ (660 W m^{-1} K^{-1}), which is comparable to the bulk silicon with strong covalent bonding interactions, can be generated by a weak van der Waals interaction. Our analysis shows that the anomalous κ arises from one-dimensional-like phonons propagating in the cross-plane direction, which is due to the extremely large phonon anisotropy induced by the combined effect of atomic-mass difference and structural anisotropy. This discovery paves an avenue to realize thermally conductive materials that have weakly bonded structures, which can be potentially applied in the design of high-performance nanoelectronic devices.

With the rapid development of miniaturization and high-power density of electronic devices, the discovery and design of materials with high thermal conductivities is critical to address future heat management challenges.[1–3] In nonmetallic solids, the lattice thermal conductivity (κ) contributed by phonons is mainly responsible for thermal transport. Typically, κ is limited by the lowest-order process arising from the anharmonicity of the interatomic potential, three-phonon scattering in crystals.[4–8] By assuming that only the acoustic phonon modes participate in thermal conduction and neglecting the phonon anisotropy,[9,10] half a century ago, Slack established a famous criterion, which states that only crystals composed of strongly bonded light elements should exhibit high κ.[11] To date, this criterion has been the one most used to connect crystal structures and atom species with macroscopic thermal conductivity.[7,12–15]

According to the Slack criterion, it is not surprising that carbon allotrope bulk crystals, such as diamond and graphite, have a record high κ of about 2000 W m^{-1} K^{-1} at room temperature.[11,16] This value is four times larger than that of SiC, which has highest measured κ among commercial semiconductors (490 W m^{-1} K^{-1}).[17] However, for commercial applications, high-quality natural diamond is scarce and expensive. Moreover, for graphite, κ is highly anisotropic, i.e., the cross-plane thermal conductivity (κ_z) is two orders of magnitude smaller than the in-plane one (κ_r) due to the weak van der Waals (vdW) interlayer interactions.[18] This feature largely limits its applications in thermal management.

Fundamentally, κ in a crystalline material is determined by mode-dependent heat capacity C, group velocity ν, and relaxation time τ as[7]

$$\kappa = \sum_{\mathbf{qs}} C_{\mathbf{qs}} \nu_{\mathbf{qs}}^2 \tau_{\mathbf{qs}}, \tag{1}$$

where the subscript $\mathbf{qs}$ denotes a phonon mode with wave vector $\mathbf{q}$ in the sth phonon branch. Note that Eq. (1) is a fundamental equation

for precisely calculating a material's thermal conductivity.[7,19–23,34] On the basis of Eq. (1), it is generally believed that a material with heavier average atomic mass (denoted as $\bar{M}$) has a smaller κ (negative atomic-mass correlation), since the larger $\bar{M}$ gives rise to lower phonon frequency and, thus, smaller phonon group velocity.[7,24–26] This derivation agrees well with the Slack criterion.[11] However, according to Eq. (1), one may also expect an increase in κ with $\bar{M}$ (positive atomic-mass correlation), provided that the relaxation time τ significantly increases with $\bar{M}$. Unfortunately, such a phenomenon has rarely been observed, because the larger $\bar{M}$ is usually accompanied by stronger phonon scattering, which decreases τ due to the scaling down of the phonon frequency.[11] Hence, exploring a new mechanism that allows high κ with both heavy elements and weak atomic interactions in solids not only can complement the long-held Slack criterion but also pave promising avenues for the design of commercial thermally conductive materials.

In this Letter, by solving the fundamental thermal conductivity equation from first-principles calculations, we reveal a thermal transport mechanism originated from the phonon anisotropy with one-dimensional-like (1D-like) phonons. Such a mechanism allows the positive atomic-mass correlation and unusual high thermal conductivity with heavy elements and weakly bonded interactions, departing from the long-held Slack's criterion.

The boron-based III–V compounds with hexagonal lattice h-BX (X = N, P, As), which have very similar geometry but significantly different atomic mass X, are ideal candidates for this study. Recently, their intriguing in-plane κ has attracted great attention,[26–31] whereas, the study of their cross-plane κ is still scarce. Here, we first perform the first-principles calculations on their atomic structure and total energy properties. Figures 1(a)–1(c) show the obtained most stable structures of h-BN, h-BP, and h-BAs, which are in AA′, AB′, and A′B stacking, respectively. As discussed below, the different stacking structures can also induce remarkable changes in κ_z.

As shown in Figs. 1(a)–1(c), the interlayer distance monotonically increases from 3.08 to 3.63 Å with X going from N to As. The interlayer distances are about two times that of B–X chemical bonds, which are 1.44, 1.85, and 1.95 Å for X = N, P, and As, respectively, showing the nature of vdW interlayer interactions in these boron compounds. We have additionally calculated the interlayer binding energy E_b of h-BX. Considering that each bulk unit cell contains two BX layers, and each layer contains a BX pair, E_b is defined as $E_b = (2E_l - E_{tot})/2$ with E_{tot} and E_l being the total energy of the bulk BX and a BX layer, respectively. As shown in Table I, for all the structures, E_b is smaller than 700 meV per BX pair, confirming the nature of vdW interlayer interactions in h-BX solids.

Figures 1(d)–1(f) show the phonon dispersions of the bulk phases of h-BX, which resemble their monolayer counterparts in the in-plane Brillouin zone along Γ–M–K–Γ paths,[26] except for the additional optical mode ZO′ appearing around 2.5 THz originated from the opposite cross-plane vibration between two BX layers.[32] It has been found that the ZO′ mode is the key bridge for interlayer phonon scattering, which results in a significant reduction in the in-plane thermal conductivity κ_r of graphite compared with graphene.[16,33] On the other hand, since we mainly focus on the cross-plane thermal conductivity κ_z, the phonon modes along the cross-plane (Γ–A) path are particularly addressed here. Note that the cross-plane LA (LO′) mode along the Γ–A path corresponds to the in-plane ZA (ZO′) mode,[32] because both of them are from the identical (opposite) cross-plane vibrations between two BX layers (see Fig. S3). As discussed below, the cross-plane LA modes have dominating contribution to κ_z.

The thermal conductivity is calculated using an *ab initio* methodology based on a density functional theory (DFT) and a solution of the phonon Boltzmann transport equation (BTE) with three-phonon processes[34] without inclusion of the four-phonon processes.[35–37] Note that, in use of this method, the calculated room-temperature κ_r of h-BN is about 500 W m^{-1} K^{-1}, which is consistent with the recent experimental observations (420–550 W m^{-1} K^{-1}).[27,30] Figure 2(a) shows the temperature dependence of thermal conductivities in both cross-plane and in-plane directions. It is seen that in the whole simulated temperature region (100–800 K), the κ_r of h-BAs is significantly smaller than that of h-BP and h-BN due to the decrease in the phonon velocity and the increase in the phonon scattering rate,[26] agreeing with Slack's criterion.[11] It is noteworthy that κ_r of h-BP is unusually large, which is comparable to that of h-BN, owing to the particular interlayer interaction effect on the in-plane phonon transport.[38]

As for the variation in κ_z, however, the converse result is obtained. κ_z of h-BP and h-BAs is much higher than h-BN, showing the larger atomic mass $\bar{M}$ corresponds to a higher thermal conductivity. This characteristic becomes more and more obvious with decreasing temperature, which results in a large discrepancy in κ_z as X goes from N to As at 100 K, i.e., κ_z of h-BAs (h-BP) reaches up to 2.8 (2.4) times that of h-BN. Such a striking enhancement of κ_z with $\bar{M}$ significantly departs from the long-held concept, that is, larger $\bar{M}$ corresponds to lower thermal conductivity.[7,11]

Another intriguing characteristic of κ_z is that thermal conductivity originating from a weak vdW interaction can be significantly higher than that from a strongly bonded interaction. As one can see from Fig. 2(b), κ_z is considerably higher than κ_r in h-BAs with κ_z/κ_r increasing from 1.5 to 2.6 as the temperature decreases from 800 to 100 K. This anomalous feature is unexpected according to the general thermal transport theorem, i.e., stronger bonded interaction gives rise to higher thermal conductivity.[7,11] On the contrary, the thermal conduction in h-BN is quite normal ($\kappa_z/\kappa_r < 0.3$), and it is in between for h-BP ($0.2 < \kappa_z/\kappa_r < 0.4$). As indicated in Fig. 2(a), the increase in κ_z/κ_r with heavier element X may be due to two facts, one is the anomalous increase in κ_z, and the other is the decrease in κ_r as generally expected. Moreover, as shown in Fig. 2(a), κ_z of h-BAs (h-BP) increases from 150 (170) to 660 (560) W m^{-1} K^{-1} as the temperature decreases from 300 to 100 K. The thermal conductivity is comparable to that of the usual thermal conductive materials with covalent bonded interactions such as bulk silicon.[39] This result shows that the thermal transport originating from weak vdW interactions can be comparable to that from strongly bonded interactions, which overcomes Slack's criterion.[11]

In Figs. 3(a)–3(c), we additionally show the projected κ_z of h-BX at 100 K on the basal plane (0 0 1) in the Brillouin zone. As one can see, in all three h-BX solids, κ_z is mostly concentrated around the Γ point in the 2D Brillouin zone. This feature shows that the cross-plane thermal transport is mostly contributed by the phonon modes along the cross-plane Γ–A path (Fig. 1). Hence, in the following discussions, we focus on the contributions of the phonon modes along the Γ–A path to κ_z. Fig. 3(d) shows the relative contributions of LA, TA, and all the optical phonon modes along the Γ–A path. It is seen that κ_z of the three BX solids exhibits distinguished phonon-mode-contribution

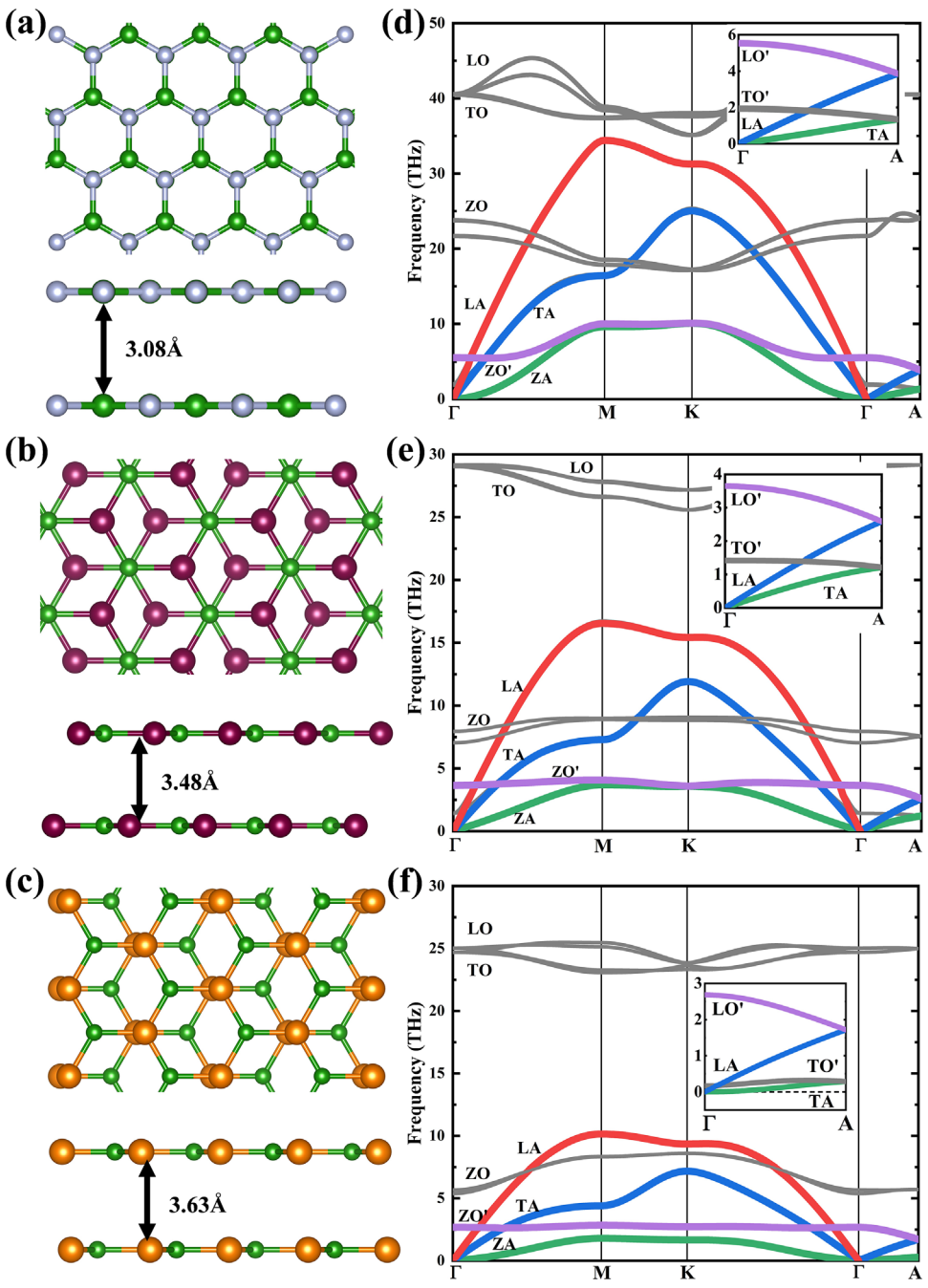

FIG. 1. (a)–(c) Optimized most stable atomic structures of h-BX with X = N, P, and As, respectively. (d)–(f) The corresponding phonon dispersions of h-BX structures in (a)–(c). (a) and (d) The results for h-BN, (b) and (e) represent the results for h-BP, and (c) and (f) represent the results for h-BAs. In (a)–(c), the green, gray, purple, and orange balls depict B, N, P, and As, respectively. The interlayer distance d_L is also shown. In (d)–(f), Γ–A corresponds to the cross-plane path, and Γ–M–K–Γ correspond to the in-plane paths in the Brillouin zone. The inset shows magnified phonon dispersions in the Γ–A path.

characteristics. For h-BN, the TA mode (contributes 69.2% to κ_z) is mainly in charge of cross-plane thermal transport. (The LA mode only contributes 25.9%.) As for h-BP, however, the contribution of the LA mode increases to 32.5% accompanied by a significant reduction of contribution from the TA mode to 63.4%. More interestingly, compared with h-BP, in h-BAs the contribution of the LA mode increases from 32.5% to 63.1%, accompanied by a substantial reduction in contribution from the TA mode (from 63.4% to 28.8%). This result reveals that the anomalous enhancement of κ_z with $\bar{M}$ in h-BX is owing to the increase in thermal conductivity contributed by the LA mode, accompanied by a reduction in thermal conductivity contributed by other phonon modes.

The frequency dependence of κ_z (Fig. S4) further shows that κ_z is mainly attributed to the low-frequency phonons, i.e., $\omega < 5$, 4, and 3 THz with X = N, P, and As, respectively. This result is consistent with the fact that the high-frequency modes (ZO, TO, LO) are hardly

TABLE I. The calculated structural parameters, interlayer binding energy E_b (meV per BX pair), and average atomic mass $\bar{M}$ (amu) of h-BX (X = N, P, and As). For the structural parameters, the in-plane lattice constant a (Å), ionic radii r of element X (Å), interlayer distance d_L (Å) as indicated in Fig. 1, and the nearest-neighbor distance between interlayer X atoms d_X (Å) are shown. Note that the Pauling ionic radius of B^{+3} is 0.20 Å.

	Stacking	a	r	d_L	d_X	E_b	$\bar{M}$
BN	AA′	2.50	1.71	3.08	3.40	677	12.5
BP	AB′	3.20	2.12	3.48	3.86	536	21.0
BAs	A′B	3.38	2.22	3.63	3.66	522	43.0

excited at 100 K [Figs. 1(d)–1(f)], which allows us to concentrate on the contributions from the low-frequency modes (TA, LA, TO′, LO′). We additionally calculated the group velocity V_g and relaxation time τ of low-frequency phonon modes along the Γ–A path, which play critical roles in determining κ_z according to Eq. (1). As shown in Fig. 4, although V_g in h-BP and h-BAs are basically 1–2 times smaller than that in h-BN, most of τ in them are larger by 10–100 times in the frequency region $\omega < 3$ THz. Considering that this frequency region coincides with that of LA modes along the Γ–A path (Fig. 1), the increase in κ_z in h-BP and h-BAs, with respect to h-BN, mainly originates from the considerably enhanced τ of the LA mode. Note that the smaller κ_z of h-BP in comparison with h-BAs is mainly attributed to the obviously smaller V_g with $\omega < 2$ THz [Fig. 4(a)].

The significantly enhanced τ of LA modes can be attributed to the phonon anisotropy with 1D-like phonons. As shown in Figs. 1(d)–1(f), in the low-frequency region along the Γ–A path, the frequency of transverse modes (TA, TO′) drastically decreases with X going from N to As due to the combined effect of the reduction in the in-plane B–X bonding strength and the increase in $\bar{M}$. This feature is especially remarkable in h-BAs, where TA and TO′ modes nearly flatly disperse and can be recognized as localized phonon modes. The flattening of transverse branches corresponds to a decrease in transverse phonon frequencies and group velocities. It is known that the scattering rate between two phonon modes is inversely proportional to the energy gap[7,26] due to the requirement of the selection rule on both energy and momentum.[6,23] The significant decrease in transverse phonon frequencies can increase the bandgap between the transverse (TA, TO′) and longitudinal (LA) phonon modes, which, thus, has an effect of reducing phonon–phonon scatterings between them at low temperatures. Therefore, the increase in X from N to P/As has an effect of decoupling the interactions between transverse and longitudinal phonon modes, making the phonon anisotropy with 1D-like phonon characteristic along the longitudinal (cross-plane) direction, which results in unusually large τ. Particularly, the flatten of TA and TO′ modes is much more profound than the LA mode in h-BAs than that in h-BN and h-BP, which leads to the sizable large bandgap and, thus, extremely large phonon τ of the LA mode. This feature makes h-BAs own the largest κ_z in the h-BX system at low temperatures.

We have further calculated the phonon density of states (PDOS) of h-BX, the magnitude of which is proportional to the number of phonons responsible for thermal transport. As shown in Fig. S5, PDOS of P and As atoms in h-BP and h-BAs are particularly dominating in the low-frequency region ($\omega < 5$ THz), different from that of h-BN. This means that the vibrations of P and As atoms are responsible for the cross-plane thermal transport. On the other hand, one can also understand this phenomenon from the geometry characteristics of h-BX. As shown in Table I, the Pauling ionic radii of B^{+3}, N^{-3}, P^{-3}, and As^{-3} are 0.20, 1.71, 2.12, and 2.22 Å, respectively. This means that the interlayer interaction between B–X atoms is very weak due to the small

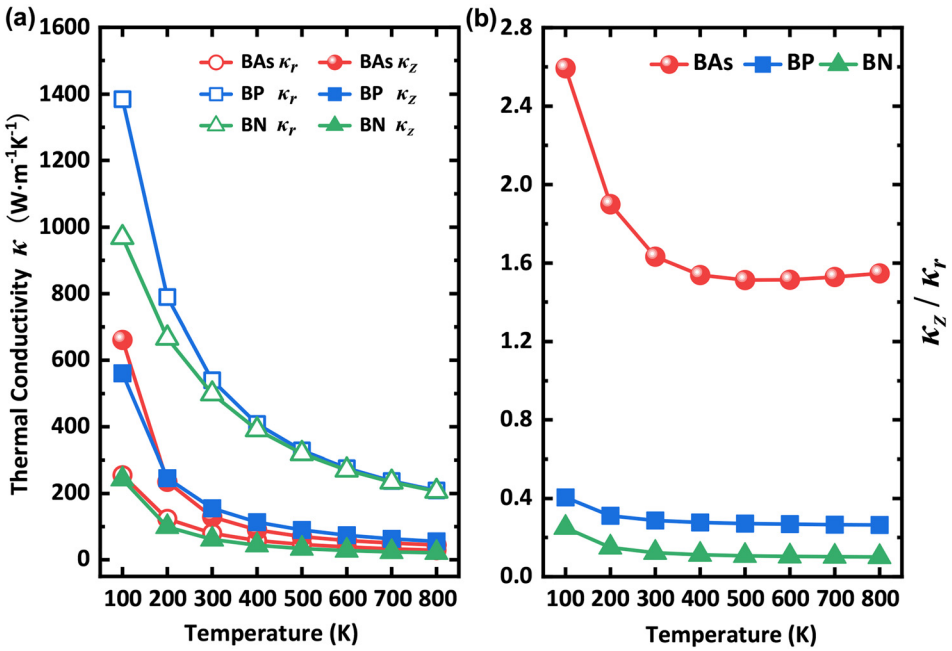

FIG. 2. (a) Calculated cross-plane thermal conductivity κ_z and in-plane thermal conductivity κ_r as a function of temperature. The solid and empty symbols represent κ_z and κ_n respectively. (b) Temperature dependence of κ_z/κ_r. The triangles, squares, and circles correspond to thermal conductivity of h-BN, h-BP, and h-BAs, respectively.

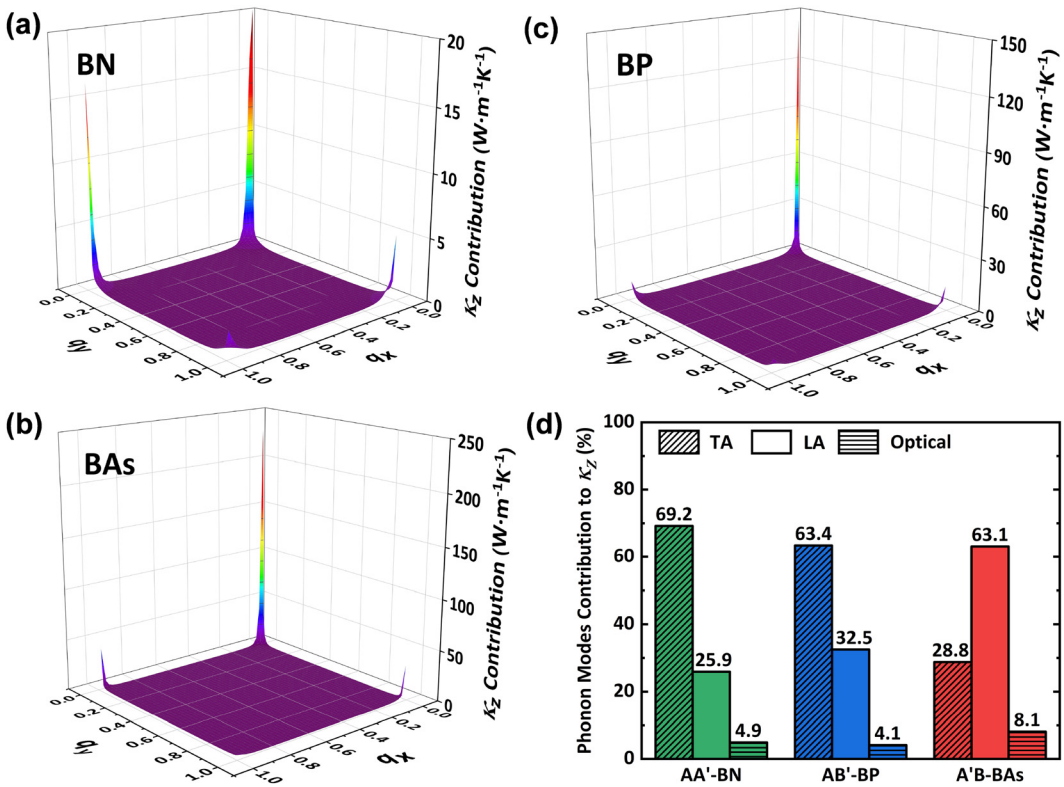

FIG. 3. (a)–(c) κ_z projected on the basal plane (0 0 1) in the Brillouin zone for h-BX with X = N, P, and As, respectively. (d) Percentage contribution to κ_z of phonon modes along the Γ–A path for h-BX (X = N, P, As). The results are obtained at 100 K.

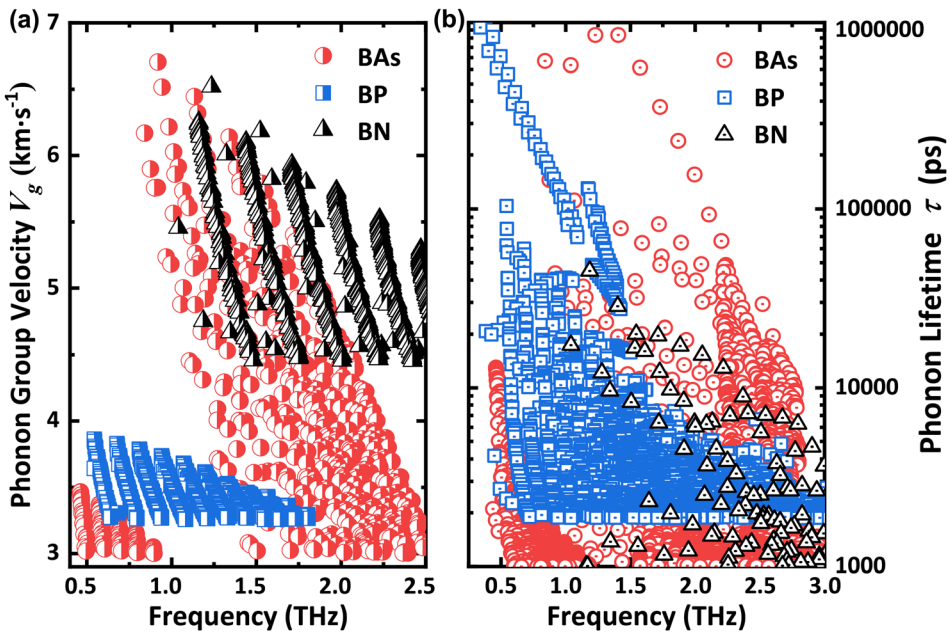

FIG. 4. (a) Group velocity V_g and (b) phonon relaxation time τ along the Γ–A path at 100 K. The triangles, squares, and circles correspond to thermal conductivity of h-BN, h-BP, and h-BAs, respectively.

radii of B^{+3}, whereas the interlayer interaction between X–X atoms is much stronger due to their considerably larger radii. Especially notable is the nearest-neighbor interlayer distance between As–As (P–P) atoms is 0.58 (0.38) Å smaller than the sum of their radii, showing that their interactions are stronger than the usual vdW ones. The above results show that cross-plane vibration of X atoms has a more dominating contribution to κ_z in h-BP and h-BAs.

From the above discussions, one can construct a one-dimensional (1D) atomic chain picture by considering the thermal conduction channels to be composed of X–X atomic chains in the cross-plane direction. Actually, the thermal conductivity of a 1D atomic chain had been widely studied in both theoretical models and computational simulations.[4,40–42] It has been found that phonon scatterings are notably weaker in 1D systems than in 3D systems, because of the quantum confinement effect, which leads to an unusually large phonon mean free path (PMFP) (proportional to τ) as well as the ultrahigh thermal conductivity.[42–47] To verify this picture, we have evaluated the maximum PMFPs[34] of h-BX with X = N, P, and As at 100 K. As shown in Fig. S6, for all the three structures, PMFPs of κ_r dominated by the 2D vibration modes converge in the range of 10^6–3×10^6 nm, significantly smaller than that of κ_z in h-BP and h-BAs (6.0×10^6–7.5×10^6 nm). Note that the PMFPs of h-BP and h-BAs are even 6.0–7.5 times larger than that of h-BN. This result confirms the unusually large PMFPs of the 1D vibration mode. Therefore, one can conclude that 1D vibrations of X–X atomic chains in the cross-plane direction are the origin of the unusually positive atomic-mass correlation and high value of κ_z in h-BX vdW solids.

Accordingly, it is natural to realize that κ_z would be dramatically influenced by the stacking structure, which directly correlates with the geometry and atomic interaction strength in the cross-plane direction. Hence, we have evaluated κ_z of h-BAs with AB′ stacking, where the 1D As–As cross-plane chains appeared in A′B stacking have been destroyed (see SVII in the supplementary material). As a result, κ_z dramatically decreases by a factor of 60 at 100 K (Fig. S7). This result confirms the picture of 1D-like phonon transport for the anomalous κ_z in h-BX structures.

In summary, we have revealed a thermal transport mechanism induced by phonon anisotropy with 1D-like phonon phonons, which allows anomalous thermal conductivity, i.e., positive atomic-mass correlation and high thermal conductivity with heavy elements and weakly bonded interactions, departing from the long-held Slack's criterion. We would like to remark that this mechanism should be general if 1D thermal conduction channels can be formed, which likely exist in materials with significant atomic-mass difference and remarkable structural anisotropy.

See the supplementary material for theoretical method and additional results corresponding to h-BX.

We dedicate this paper to Dr. Hao Wu, who unfortunately passed away before the work finished. Hao initialized this work and performed most calculations. He is greatly missed. We are grateful for useful discussions with Professor Tao Ouyang and Professor Zhibin Gao. Z.-X.G. acknowledges funding support from the National Natural Science Foundation of China (No. 12074301). Calculations were performed at the Supercomputer Center of Fudan University.

AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Hao Wu: Data curation (equal); Investigation (equal); Methodology (equal). **Yi-Lin zhang:** Data curation (equal); Investigation (equal); Methodology (equal). **Zhi-Xin Guo:** Formal analysis (equal); Writing – original draft (equal); Writing – review & editing (equal). **Xin-Gao Gong:** Conceptualization (lead); Formal analysis (equal); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

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