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Negative thermal expansion of group III-Nitride monolayers

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Abstract

Materials with a negative thermal expansion coefficient have diverse potential applications in electronic engineering. For instance, mixing two materials with negative and positive thermal expansion coefficients can avoid changing volume with temperature. In this study, we investigate the variation of linear thermal expansion coefficients (LTECs) of group III-Nitride monolayers (h-XN, where X = B, Al, Ga, In) with temperature using quasi-harmonic approximation. We also explore phonon thermal properties of h-XN monolayers, including specific heat, entropy, and free energy. These systems are revealed to exhibit considerably high negative LTEC values below the room temperature. To understand the origin of negative thermal expansion, we analyze the contribution of individual phonon branches to the LTEC, and it is found that the highest contribution is originating from ZA (out-of-plane acoustic) phonon mode. While h-BN and h-AlN monolayers exhibit negative LTEC values converge to the zero for h-GaN and h-InN monolayers above room temperatures. These findings can be crucial in designing h-XN based nanoscale heat devices.

Keywords: thermal expansion, nitrides, Grüneisen parameter

(Some figures may appear in colour only in the online journal)

1. Introduction

Following the isolation of graphene [1] and the discovery of other monolayer systems [2], the two-dimensional (2D) family has expanded rapidly, enveloping a variety of compositions [3]. Among them, 2D group III-Nitrides (BN, AlN, GaN, InN), which share similar structural characteristics with graphene, stimulated particular interest [4]. In these systems, group III elements and nitrogen atoms form planes bound by sp² orbital hybrids, resulting in a honeycomb structure. The layers of these materials share some of the traits originating from the 2D nature of graphene, and layers are bound

together by dispersive interlayer forces [4–6]. However, unlike graphene, 2D group III-Nitrides are wide band gap semiconductors and exhibit different electronic and optical properties. The single layers of BN have been exfoliated from its bulk structure right after graphene by using a micromechanical cleavage method and shown to be stable under ambient conditions [7]. While after this achievement, epitaxial growth of ultrathin AlN sheets [8–10], and migration-enhanced encapsulated growth of 2D GaN [11] have also been reported. In addition, there have been various studies focusing on monoor multiple-layers of group III-Nitrides, predicting their possible forms and unveiling their unique features [4, 5]. 2D group III-Nitrides in their graphene-like planar hexagonal form are considered as ideal semiconducting materials that hold promise for high temperature electronic and optical applications

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such as light-emitting diodes, lasers, and field-effect transistors [4, 12]. These systems can be functionalized by doping [13–15] and their band gaps can be tuned by alloying and strain engineering [16–21]. Theoretical studies have also indicated that electronic properties of 2D group III-Nitrides can be modified for specific applications by heterostructure designs [22–27].

Another important facet of 2D materials, including III-Nitrides is their thermal properties [28–32], specifically unusual thermal expansion characteristics. Thermal expansion is the change in the volume (area) of a material with temperature and is an anharmonic feature related to the variation of the phonon spectrum. While most of the materials expand upon heating over a broad range of conditions, negative thermal expansion (thermal contraction) has been reported for various 2D materials with the increase in temperature [33, 34]. For instance, theoretical calculations have predicted negative linear thermal expansion coefficient (LTEC) for graphene, silicene, germanene, and phosphorene [35-37] and several theories have been suggested to reveal the possible mechanisms [38]. Various experimental studies have verified this feature for graphene in the temperature range of 300-400 K and reported LTEC values as $(-8\pm1)\times10^{-6}~K^{-1}$ at room temperature [39, 40]. However, we should note that the negative LTEC value does not limited to low dimensionality of the materials. It is related to the competition of the out-of-plane bending modes and the in-plane stretching vibration modes in the materials. For instance, graphite has negative LTEC values up to 673 K for a (in plane) lattice direction due to the dominate bending modes while it has positive LTEC values for c lattice direction [41]. In addition, negative LTEC values have been obtained in a range of solids including zeolites, polymers and complex metal oxides [42–44].

2D materials with negative LTEC can be used in composite systems as thermal expansion compensators [45]. The thermal expansion control can also widen possibilities to design nanoscale devices that can operate without expansion/ contraction across a required temperature range [46]. With this respect, understanding the thermal expansion features of 2D III-Nitrides is crucial for potential applications. With this motivation, we investigate the thermal expansion of the 2D group-III nitrides (h-BN, h-AlN, h-GaN, h-InN) by firstprinciples methods based on density functional theory (DFT). Following the optimization of monolayers, the phonon dispersion relations, LTEC values, and Grünesien parameters are obtained. We find that all 2D group III-Nitride monolayers possess negative LTEC, and it is correlated with Grünesien parameter of the transverse acoustic modes. Our calculations show that the maximum value of the LTEC increases from h-BN to h-InN while the temperature at which negative LTEC is significant decreases.

2. Computational details

The thermal properties of h-XN (X = B, Al, Ga, In) monolayers were obtained by using DFT and density functional perturbation theory (DFPT) [47–49] as implemented in the Vienna ab initio Simulation Package (VASP) [50, 51]. For the exchange-correlation potential, the Perdew-Burke-Ernzerhof (PBE) functionals [52] within generalized gradient approximation were used. A kinetic energy cut-off of 750 eV was used with Γ -centered k-point grids of $32 \times 32 \times 1$ for primitive cell [53]. Phonon dispersion curves were determined by using PHONOPY code [54] interfaced with the VASP [55] for the 4 \times 4 \times 1 supercell with Γ -centered 8 \times 8 \times 1 k-point mesh and displacement of 0.01 Å from the equilibrium atomic positions. We considered a 20 Å thick vacuum layer along the zaxis to avoid interactions between the neighboring layers. The convergence criterion for the total energy was set as 10^{-5} eV, and 10^{-8} eV for the optimization and phonon calculations, respectively. A maximum force of 0.0002 eV Å⁻¹ was allowed on each atom. We used PHONOPY results of thermal properties to calculate LTECs and Grüneisen parameters under the quasi-harmonic approximation (QHA) [56].

It is noted that the Helmholtz free energy F is dominated by the ground-state energy and the vibrational free energy. Thus, the contribution of the phonon to free energy is expressed as follows:

$$F_{\nu ib} = \frac{1}{2} \sum_{q,\nu} \hbar \omega_{q,\nu} + \kappa_B T \sum_{q,\nu} \ln[1 - \exp(-\hbar \omega_{q,\nu}/(\kappa_B T))].$$
(1)

Here, q and v stand for the wave vector and the band index, respectively. $\omega_{q,v}$ represents the vibrational frequency at q and v. T, κ_B , and \hbar denote the temperature, Boltzmann constant, and reduced Planck constant, respectively. The heat capacity (C_V) and the entropy (S) at constant volume were evaluated from equations (2) and (3), respectively, as follows:

$$C_{V} = \sum_{q,v} \kappa_{B} \left(\frac{\hbar\omega_{q,v}}{\kappa_{B}T}\right)^{2} \frac{\exp\left(\frac{\hbar\omega_{q,v}}{\kappa_{B}T}\right)}{\left[1 - \exp\left(\frac{\hbar\omega_{q,v}}{\kappa_{B}T}\right)\right]^{2}}$$
(2)
$$S = \frac{1}{T} \sum_{q,v} \frac{\hbar\omega_{q,v}}{\left[\exp\left(\frac{\hbar\omega_{q,v}}{\kappa_{B}T}\right) - 1\right]}$$
$$- \kappa_{B} \sum_{q,v} \ln[1 - \exp(-\hbar\omega_{q,v}/(\kappa_{B}T))].$$
(3)

The heat capacity at constant pressure (C_P) was then evaluated as

$$C_P = \frac{T\partial^2 G(T,P)}{\partial T^2} = \frac{T\partial V(T,P)}{\partial T} \frac{\partial S(T,V)}{\partial V} + C_V[T,V(T,P)]$$
(4)

where G is the Gibbs free energy which is defined as

$$G(T,P) = min_V[U(V) + F_{vib}(T,V) + PV].$$
(5)

In equation (5), V represents the equilibrium volume at T and P. The thermodynamic properties at constant pressure were obtained from the data set of U(V) and F_{vib} at a given volume range. The fact that 2D materials have a very soft

out-of-plane transversal acoustic mode, the volume was carefully estimated within a small applied strain range. For this, we applied the in-plane strain in the range of $\pm 0.5\%$ for successive $\pm 0.1\%$ step corresponding to the lattice parameters of the h-XN monolayers. This is to avoid negative modes near the Γ point that can invalidate QHA calculations. It should be noted the translational and rotational invariants are not imposed on force constants of the considered h-XN monolayers. The data set obtained from equation (5), then fitted into the Birch–Murnaghan state equation to evaluate the temperaturedependent LTEC (α (T)) for 2D materials, which is given as

$$\alpha(T) = \frac{1}{a(T)} \frac{\partial a(T)}{\partial (T)} = \frac{1}{2V} \frac{\partial V}{\partial T} = \beta_T B_{2D}^{-1}$$
(6)

where $\alpha(T)$ indicates the change of volume (area) at a given temperature for a minimum of Gibbs free energy, *a* is the crystal lattice constant. In equation (6), the B_{2D} is the bulk modulus and the β_T is the thermal tension which is given by

$$\beta_T = \frac{1}{A_{2D}N} \sum_{q,v} \gamma(q,v) \frac{\partial E(w(q,v),T)}{\partial T}$$
(7)

where A_{2D} is the area of the unitcell, N is the number of unitcells within the crystal, E(w(q,v),T) is the vibrational energy of phonons and the $\gamma(q,v)$ is the Grüneisen parameters and given as

$$\gamma(q, v) = -\frac{1}{w}(q, v) \sum_{i} \frac{\partial w(q, v)}{\partial \epsilon_{ii}}.$$
(8)

More details related with the calculation of LTEC can be find in the literature [57–59]. The thermal properties of a material are correlated with phonon modes and electronic excitations. However, it should be noted that h-XN monolayers are wide band gap semiconductors, which means phonon modes dominate thermal property. We can therefore exclude the contribution of electronic excitation to thermal property as their band gaps would be greater than the excitation energy.

3. Results and discussion

The optimized crystal structures of h-XN (X = B, Al, Ga, and In) monolayers are illustrated in figure 1 and the calculated structural parameters listed in table 1. The obtained results are compatible with the literature [5, 14].

The obtained phonon dispersion curves for the equilibrium structures along the high symmetry directions of the Brillouin zone (BZ) are given in figure 2(a). None of the phonon dispersion curves has imaginary frequencies in the whole BZ. These honeycomb structures have six vibrational phonon modes, including three acoustic (in-plane longitudinal acoustic mode (LA), transverse acoustic mode (TA), and out-of-plane transverse acoustic mode (ZA), and three optical branches. As shown in figure 2(a), in the vicinity of Γ -point, the ZA branch has a quadratic form while the LA and TA branches show linear dispersion which is well known feature in phonon dispersions of the 2D materials.



Figure 1. A sample crystal structure of h-XN in top view. The unitcell is illustrated with solid lines. The green and grey balls represent X (B, Al, Ga, In) and N atoms, respectively.

Table 1. Optimized lattice parameters (a) of h-XN monolayer structures. The values in parentheses are obtained from Birch–Murnaghan equations of state fit. Bond length (d) between the X and N, charge transfer (Q) from group-III atoms to the N atom, the electronegativity difference ($\Delta \chi = \chi_N - \chi_X$) by Pauling scale ($\chi_N = 3.04$) are given.

	a (Å)	d (Å)	Q (e ⁻)	$\Delta \chi$
h-BN	2.5123 (2.5129)	1.450	2.18	1.00
h-AlN	3.1259 (3.1274)	1.805	2.30	1.43
h-GaN	3.2542 (3.2574)	1.879	1.33	1.23
h-InN	3.6372 (3.6383)	2.099	1.21	1.26

The Gibbs free energy (G), entropy (S), and heat capacity (C_v) as a function of temperature for h-XN systems are displayed in figures 2(b). The G, S, and C_{ν} exhibit similar features for all the considered h-XN monolayers at high temperatures. However, they show dramatic changes, especially at temperatures below 400 K. For instance, while h-BN has positive free energy in the whole range from 0 to 1000 K, h-AlN, h-GaN, and h-InN have negative free energy after 600, 400, and 250 K, respectively, which may indicate the energetic instability of these monolayers for high temperatures. Compatible with these free energy values, the entropy of the h-XN monolayers increases with temperature as expected, and the highest (lowest) entropy value is obtained for h-InN (h-BN). Lastly, in accordance with the third law of thermodynamics, the heat capacity of h-XN monolayers depends on temperature, and C_{v} approaches to zero as temperature decreases. At high temperatures, C_{ν} converges to the Dulong-Petit limit (3NR, where N indicates the number of atoms in the unit cell). The obtained results for h-BN are in good agreement with the literature [34, 60].

Thermal expansion is the tendency of matter to change its area, volume, and shape in response to a variation in temperature, and knowing the LTEC of materials is one of



Figure 2. (a) Phonon dispersion curves and (b) temperature dependent Gibbs free energy (G), entropy (S), and heat capacity (C_{ν}) of h-XN monolayers.



Figure 3. (a) LTEC and (b) the calculated mode Grüneisen parameters as a function of temperature for h-XN monolayers.

the important physical quantities that can be used to examine material's suitability for heat management in a device.

Therefore, here, we present our findings on the LTEC of h-XN monolayers. As mentioned above, we performed OHA calculations within a small strain range to ensure the occurrence of non-negative phonon modes in the vicinity of Γ -point. Temperature-dependent LTECs of h-XN monolayers are illustrated in figure 3(a). It is notable to emphasize that LTECs values converge to zero for h-AlN, h-GaN, and h-InN monolayers for elevated temperatures except for h-BN monolayer. It should be noted that LTEC curves initially decrease with increasing temperature until a minimum value has been reached and then increases rapidly until convergence to zero has been reached. The estimated minimum LTECs values are $-14.5 \times 10^{-6} \text{ K}^{-1}$ @ 200 K for h-BN, $-25.5 \times 10^{-6} \text{ K}^{-1}$ @ 80 K for h-AlN, $-48.7 \times 10^{-6} \text{ K}^{-1}$ @ 110 K for h-GaN and $-79~\times~10^{-6}~K^{-1}$ @ 30 K for h-InN. These negative LTEC values of the h-XN monolayers differ from their bulk counterparts. For example, h-BN has positive thermal expansion $(37.7 \times 10^{-6} \text{ K}^{-1} \text{ at } 297.5 \text{ K})$ in the c-direction, but due to the anisotropic bond strength between the interlayer and intralayer of BN, in the a-direction negative thermal expansion value with -2.72×10^{-6} K⁻¹ at 297.5 K is obtained experimentally [61]. The maximum thermal expansion coefficients obtained for bulk AlN in the range of 300–1100 K are 5.3×10^{-6} K⁻¹ and 4.2×10^{-6} K⁻¹ along the a and the c axes, respectively [62] while these values are 5.6×10^{-6} K⁻¹ and 4.8×10^{-6} K⁻¹ for bulk GaN [63] and 4.1×10^{-6} K⁻¹ and 2.9×10^{-6} K⁻¹ for bulk InN [64].

The sign of the thermal expansion is related to the anharmonic couplings between the in-plane stretching vibration modes and out-of-plane bending modes in the materials. The negative LTEC values are obtained when the out-of-plane bending modes become dominant with respect to the inplane stretching vibration modes. As is well known, phonon dispersion has optical and acoustical branches and optical branches has high frequencies, so they do not give much contribution to the thermal properties of the materials. On the other hand, the acoustical branches with low frequency mainly determine the thermal response of the system. Among the acoustical branches, especially the out-of-plane acoustic (ZA) branches give the dominant contribution to the thermal expansion coefficient of the materials. This phenomenon is well known and extensively studied for various 2D materials [57–59, 65–67]. As can be easily seen from the equations (6)–(8) that the $\alpha(T)$ is directly proportional to the thermal (β_T) tension and the β_T is related to the Grüneisen parameters. Accordingly, the Grüneisen parameters have an important role in thermal expansion mechanisms. Figure 3(b) shows the Grüneisen modes of h-XN monolayers in the whole BZ and as can be seen while almost all parameters have positive values, $\gamma(q)$ has large negative values for specific q interval values which are related to the lowest acoustic mode (ZA). Consequently, due to these dominant large negative $\gamma(q)$ modes the LTEC values of h-XN monolayers becomes negative at low temperatures.

As is seen from the LTEC curve of h-BN (figure 3(a)), the thermal contraction has its minimum temperature in an interval (0-200 K), then reaches a maximum near 800 K. Our estimated temperature range for minimum LTEC of h-BN monolayer is in accordance with those reported in the literature [34, 60, 68]. The trend of LTEC curves for h-AlN and h-GaN monolayers are almost similar, and their minimum LTEC values are obtained ~ 80 and ~ 110 K, respectively. Beyond these temperature values, the LTEC curves increase monotonically and converge to zero after 400 K. The variation of h-InN LTEC with temperature is similar to that of h-GaN and h-AlN. However, the minimum LTEC value of the h-InN $(-79 \times 10^{-6} \text{ K}^{-1})$ is obtained at ~30 K, and it converges to zero faster (at around 100 K and above) than other systems. Accordingly, it can be deduced that the thermal contraction of the h-InN monolayer is more pronounced than that of the h-XN (X = B, Al, Ga) monolayers. As it is pointed out that the minimum value of LTEC decreases from h-InN to h-BN. This trend is also related to the Grüneisen parameters. At low temperatures, the optical modes are not excited due to their relatively high frequency values. However, the lower frequency acoustic modes can be excited easily. When we compare the Grüneisen parameters which are related to the ZA modes of the h-XN monolayers, h-InN has the largest negativity. The order of negativity for $\gamma_i(q)$ modes from more negative to the less negative is h-InN > h-AlN > h-GaN > h-BN. This order is also similar to variation of the minimum LTEC values. These two analogous trend imply that the lowest acoustical modes can be excited at lowest temperature value.

However, we should also note that the minimum LTEC value decreases from h-InN to h-BN, which is different from the trend at room temperature. The room temperature thermal expansion values for h-BN, h-AlN and h-GaN are $-12 \times 10^{-6} \text{ K}^{-1}$, $-5 \times 10^{-6} \text{ K}^{-1}$ and $-3 \times 10^{-6} \text{ K}^{-1}$, respectively while h-InN LTEC converges to zero. Recently, Cai et al experimentally measured the thermal expansion coefficient of the monolayer BN and the estimated LTEC values are -3.58×10^{-6} K⁻¹ and -5.1×10^{-6} K⁻¹ at room temperature [65, 66]. Our calculated LTEC value of h-BN at room temperature is almost 2-3 times larger than the experimental results. The difference between these values can be related to the limitation of the exchange-correlation functional in representation of the fundamental vibrational modes [67] and also linked to the selected supercell size for phonon calculations (finite size effect) [57].

Negative LTEC values indicate thermal contraction, which can be important in developing composite materials for temperature-dependent volume applications by mixing h-XN monolayers with other 2D materials that have positive LTEC. For instance, the volume or area of the heterostructure formed with h-XN/2D does not change with temperature variation can provide stability of electronic features of the devices.

4. Conclusion

In summary, we have theoretically studied the vibrational and thermodynamic properties of h-XN monolayers using DFPT within QHA at the level of PBE. h-XN monolayers are dynamically stable and are wide band gap semiconductors. Our findings show that the LTEC for all h-XN monolayers has negative values for certain temperatures (0-800 K) different from their bulk counterparts [61, 63, 64, 69]. The lowest LTEC are found to be $-14.5 \times 10^{-6} \text{ K}^{-1}$ @ 200 K for h-BN, $-25.5 \times 10^{-6} \text{ K}^{-1}$ @ 80 K for h-AlN, $-48.7 \times 10^{-6} \text{ K}^{-1}$ @ 110 K for h-GaN and $-79\ \times 10^{-6}\ K^{-1}$ @ 20 K for h-InN. The negative trend of LTECs has continued at room temperature for h-BN with a significant LTEC, but getting smaller for h-AlN and h-GaN. In general, the results show that the h-XN monolayers have a thermal contraction that extends around room temperature. However, LTEC approaches to zero with increasing temperature for h-XN monolayers other than h-BN. Negative thermal expansion is mainly dominated by ZA (outof-plane acoustic) phonon mode. This is validated analyzing the Grüneisen parameter, where the ZA mode largely occupied the negative Grüneisen parameter compared to other (planar) modes at low temperatures. These findings can serve as a guide for the design of nanoscale heat devices based on wide band gap semiconductors.

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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