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Molecular dynamics study on the dependence of thermal conductivity on size and strain in GaN nanofilms

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The thermal conductivity of GaN nanofilm is simulated by using the molecular dynamics (MD) method to explore the influence of the nanofilm thickness and the pre-strain field under different temperatures. It is demonstrated that the thermal conductivity of GaN nanofilm increases with the increase of nanofilm thickness, while decreases with the increase of temperature. Meanwhile, the thermal conductivity of strained GaN nanofilms is weakened with increasing the tensile strain. The film thickness and environment temperature can affect the strain effect on the thermal conductivity of GaN nanofilms. In addition, the analysis of phonon properties of GaN nanofilm shows that the phonon dispersion and density of states of GaN nanofilms can be significantly modified by the film thickness and strain. The results in this work can provide the theoretical supports for regulating the thermal properties of GaN nanofilm through tailoring the geometric size and strain engineering.

Keywords: molecular dynamics simulation, GaN nanofilm, thermal conductivity, phonon properties, size effect, strain effect

PACS: 65.80.–g, 63.22.–m, 44.10.+i **DOI:** 10.1088/1674-1056/acbf26

1. Introduction

With the rapid development of electronic technology, the performance of the first- and second-generation semiconductors cannot perfectly satisfy certain needs of modern electronic products. GaN materials, as one kind of the typical representatives of third-generation semiconductor materials, can be usually used in the electronic devices working in harsh environments due to the excellent properties of third-generation semiconductors such as high-temperature resistance, high thermal conductivity, wide band gap, and radiation resistance.[1–3] In recent years, GaN-based electronic devices have been widely used in aerospace, communication equipment, medical, and other fields,[4,5] such as power amplifiers of radar, fast charging chargers of mobile phones. In particular, GaN-based high electron mobility transistors (HEMTs) are often used in high-power devices, and the massive heat often accompanies with the working devices.[6–8] Therefore, it is necessary to quantitatively study the thermal conductivity of GaN materials to improve the performance of GaN-based power electronic materials.[9,10]

In the recent decades, there are plenty of works carried out experimentally and theoretically to study the thermal conductivity of GaN materials.[11–18] In experiments, Luo *et al.*[11] measured the thermal conductivity of GaN films grown by metal-organic chemical vapor deposition (MOCVD) at room temperature is around the range of 153 W/mK to 159 W/mK, which is higher than that of reported GaN bulk single crystal. Beechem *et al.*[12] used the time-domain thermal reflection method to obtain the thermal conductivity of doped GaN film with a thickness of 3 μm–4 μm. They found that the thermal conductivity of n-type doped GaN film was stable at 180 W/mK, and the thermal conductivity of p-type doped GaN films decreased from 160 W/mK to 110 W/mK. Ziade *et al.*[13] measured the thermal conductivity of GaN thin films with a thickness of 15 nm to 1000 nm grown on 4H–SiC without a transition layer and used the phonon transport model to explain the size dependent thermal conductivity of the GaN thin films. Jezowski *et al.*[14] measured the thermal conductivity of n-type GaN single crystal sample grown under high pressure, and found that the maximum thermal conductivity is about 1600 W/mK at 45 K and 220 W/mK at 300 K. Based on the molecular dynamics (MD) simulations, Kawamura[15] calculated the thermal conductivity of GaN bulk at 300 K in the range of 310 W/mK to 380 W/mK, and the thermal conductivity performed a downward trend with the temperature from 300 K to 1200 K. Zou *et al.*[16] found that the increase in doping concentration leads to the decrease of the thermal conductivity in GaN films. Jung *et al.*[17] identified that the thermal conductivity of GaN nanowires decreased with the increase of tensile deformation. Zhu *et al.*[18] applied the modified acoustoelastic model to predict the thermal conductivity of GaN nanofilms varied with the temperatures, stress fields,

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and thickness. It is found that the lower temperature, the thicker film, and the higher compressive stress can improve the phonon thermal conductivity in GaN nanofilms.

The GaN-based nanofilms have a great number of applications in nanoelectronic devices.[19,20] The GaN-based heterostructures will induce the mismatch stress and thermal stress in electronic devices.[21] Here, the MD simulations are performed to quantitatively explore the thermal conductivity of GaN nanofilms under various different temperatures, thicknesses, and strains, especially focusing on analyzing the dependence of thickness and strain on the thermal conductivity and phonon properties in GaN nanofilms.

2. Simulation method

The MD method[22] is used here to calculate the thermal conductivity of GaN nanofilms, which is carried out by virtue of the open-source MD simulation software LAMMPS.[23] The classical Stillinger Weber (SW) potential[24] is adopted to describe the atomic interaction in GaN structure. Note that the thermal properties simulated from SW potential can agree well with the experimental measurements.[25] This potential is composed of two-body and three-body potential. The two-body potential is determined by the distance between atoms, while the three-body potential is determined by the distance between atoms and the bond angle.

The main approach to calculate the thermal conductivity by MD simulation is usually divided into two categories: equilibrium molecular dynamics (EMD) simulation and non-equilibrium molecular dynamics (NEMD) simulation. The NEMD bases on the Fourier heat conduction law[26] and the EMD bases on the Green–Kubo formula.[27] The EMD method is used here to simulate the thermal conductivity which can directly solve the heat flow autocorrelation function. The thermal conductivity of Green–Kubo formula can be expressed as[28]

$$\kappa_x = \frac{1}{k_{\mathrm{B}} T^2 V} \int \langle J_x(t) J_x(0) \rangle \, \mathrm{d}t, \tag{1}$$

where k_{B} is the Boltzmann constant, T is the system temperature. V is the system volume. $\langle J_x(t) J_x(0) \rangle$ is the autocorrelation function of average heat flow, which is time dependent. $J_x(t)$ is the heat flow in the x direction. The mathematical expression for calculating heat flow is given as[28]

$$J_x = \frac{1}{V} \left(\sum_i e_i v_{xi} - \sum_i S_{xi} v_{xi} \right), \tag{2}$$

where e_i is the total energy of the i-th atom, v_{xi} and S_{xi} are the speed and stress of the i-th atom in the x direction, respectively.

The GaN film models with the thickness of 2 nm, 4 nm, 6 nm, 8 nm, and 10 nm are shown in Fig. 1. All the models are the supercell of wurtzite GaN with a 4-atoms primitive cell to make sure the nanofilm as the single crystal material. To simulate the thermal conductivity of GaN films, a free boundary is set up in z direction and periodic boundaries are set up in xy plane. The time step is set to 0.5 fs, and the initial models are firstly relaxed in the isobaric–isothermal ensemble (NPT) for 300 ps. Then the micro-canonical ensemble (NVE) is utilized to calculate the thermal conductivity, so as to keep the atomic number, volume, and total energy of the system unchanged. The total simulation duration is 6 ns. The average heat flow autocorrelation function is calculated every 3 fs and the value of thermal conductivity is counted every 300 ps. The final thermal conductivity is achieved by a statistical average of 20 times.

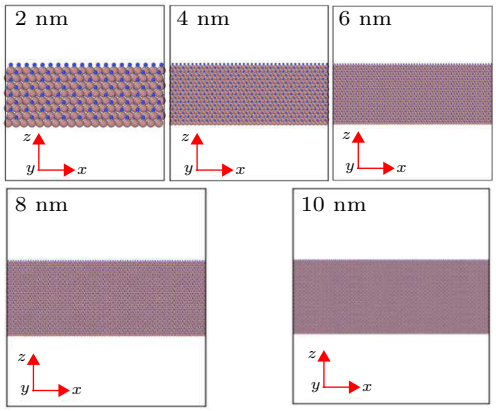


Fig. 1. GaN nanofilm model with different thickness.

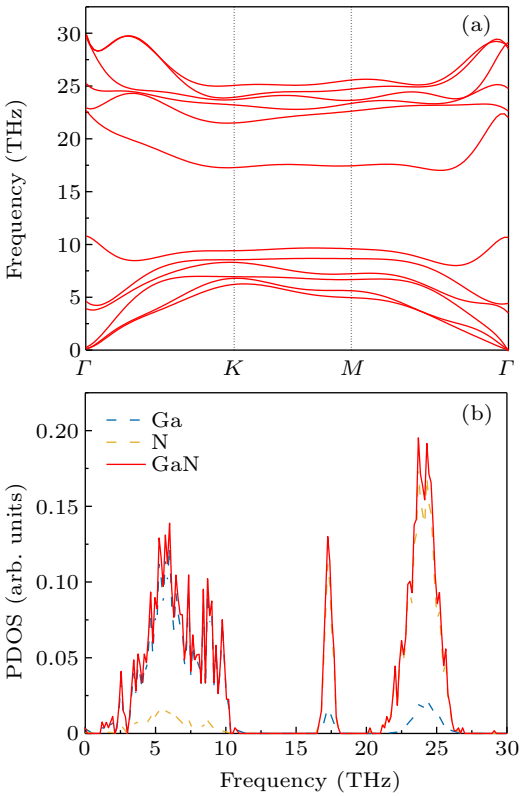


Fig. 2. Phonon dispersion (a) and phonon density of state (b) of 2 nm GaN nanofilm at 300 K.

Owing to the thermal conductivity of GaN is sensitive to the phonon properties, the fix-phonon package developed by

Kong[29] in LAMMPS is applied to calculate the binary file containing the kinetic matrix data. Then, the phonon dispersion and phonon density of states can be obtained by the post-processing software. Here, the phonon properties of primitive cell in nanofilms are given to explore the size and strain effects on the phonon dispersion and phonon density of state. The GaN phonon dispersion curves for the primitive cell in nanofilms show that there is a large band gap between the low and high-frequency branches (Fig. 2(a)), which is due to the large mass difference between the Ga and N atoms.[30] Figure 2(b) shows the phonon density of states varies with the phonon frequency of GaN, where the N atoms mainly contribute to the high-frequency optical branches above the band gap, and the low-frequency acoustic branches below the band gap are mainly contributed by Ga atoms.[31,32]

3. Results and discussion

3.1. Size effect on thermal conductivity and phonon properties

In this subsection, the thermal conductivity of GaN films with varying thickness is simulated and analyzed in detail. Figure 3(a) depicts the calculated thermal conductivity varied with the temperature for the GaN nanofilms with the thickness of 2 nm, 4 nm, and 6 nm at 200 K–1000 K based on the simulation environment described in Section 2. One can find from Fig. 3(a) that the thermal conductivity of GaN nanofilms with different thicknesses tends to decrease as the temperature rises from 200 K to 1000 K. It is due to the fact that when the temperature is higher, the number of high-frequency phonons increases, and the number of low-frequency phonons decreases, leading to a decrease in thermal conductivity.[33] It is also noted from Fig. 3(a) that the thinner the film, the temperature effect is weaker. Moreover, the variation of thermal conductivity of GaN films with thickness varying from 2 nm to 10 nm at the different temperatures of 300 K, 500 K, and 800 K, is shown in Fig. 3(b). It can be seen that the thermal conductivity increases with increasing the thickness of the film, and the thermal conductivity is approximately linear with the thickness in the range of 2 nm–10 nm. It can also be found from Fig. 3(b) that the gradient of the curves varies at different temperatures, indicating that the size dependence of thermal conductivity is sensitive to the temperature in GaN nanofilms.

Since the thermal conductivity of GaN nanofilms associates with the phonon properties, the phonon density of states (PDOS) and the phonon dispersion relationship of GaN nanofilms with the thickness of 2 nm and 8 nm are shown in Figs. 4(a) and 4(b), respectively. From Fig. 4(a), it can be noticed that the thicker GaN film has more concentrated high-frequency of phonon and lower high-frequency PDOS, along with less concentrated low-frequency of phonon and

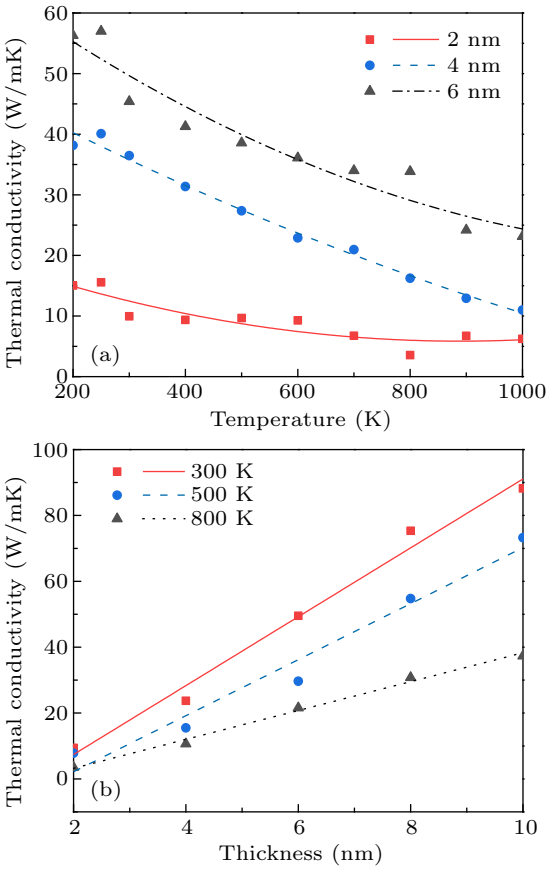


Fig. 3. The thermal conductivity of GaN films varies (a) with temperature for different thicknesses, and (b) with thickness for different temperatures.

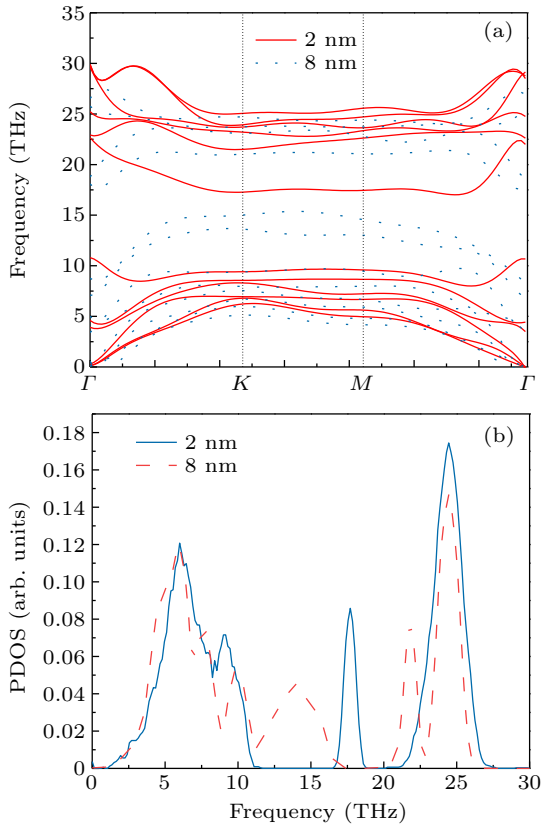


Fig. 4. Phonon dispersion (a) and phonon density of states (b) of GaN nanofilms with the thicknesses of 2 nm and 8 nm at 300 K.

higher low-frequency PDOS. It is well-known that the contributions of phonons to materials properties such as the thermal, electrical and optical properties, are related to the phonon frequencies[34,35] and the phonon scatterings.[36–38] In general, higher frequency phonons tend to have a lower mean free path and a higher rate of anharmonic scattering, which can result in a lower thermal conductivity. One can clearly find from Fig. 4(a) that the high-frequency PDOS of 2 nm GaN film is higher than that of 8 nm GaN film. Thus, the thicker GaN nanofilm with a high-frequency PDOS shows the lower thermal conductivity because of the higher rate of anharmonic scattering. Moreover, the gradient of the phonon dispersion curve of the 8 nm GaN film near the Γ point is also larger (Fig. 4(b)), indicating that its higher group velocity leads to the larger thermal conductivity.[39]

3.2. Tensile strain effect on thermal conductivity and phonon properties

Since the GaN films usually perform the elastic deformation when applying stress/strain engineering to tune the thermal performance of GaN-based devices, the thermal conductivity of GaN nanofilms with three different thicknesses (2 nm, 4 nm, and 8 nm) is simulated with the tensile strain varied from 0% to 8%. Figure 5(a) shows the variation of thermal conductivity with the strain for the GaN nanofilms with the thickness of 2 nm, 4 nm, and 8 nm at 300 K. It can be seen that the thermal conductivity of GaN nanofilms can be modified by strain engineering. As the strain increases from 0% to 8%, the thermal conductivity of GaN nanofilms with three different thicknesses (2 nm, 4 nm, and 8 nm) is decreasing. For example, the thermal conductivity of the unstrained 2 nm film is around 9.44 W/mK, while it decreases to 4.87 W/mK at a strain of 8%, with a decrement of 48.4%. It can also be seen from Fig. 5(a) that the gradients of the three curves increase with the increase of nanofilm thickness. It means that the sensitivity of strain effect on the thermal conductivity of GaN nanofilms can be tailored by film thickness design. The thermal conductivity of GaN films as the function of the strain under three different temperatures is also investigated (Fig. 5(b)). It can be found that the gradient of the curve for 300 K is the largest, and the gradient decreases with increasing the temperature. It means that the lower the temperature, the more significant the strain effect on the thermal conductivity of GaN nanofilms.

Here, the GaN nanofilm with the thickness of 4 nm is given as an example to explore the strain effect on PDOS and dispersion relations. The comparisons of the PDOS and dispersion curves of GaN film with and without strain are shown in Figs. 6(a) and 6(b), respectively. Note that the low-frequency acoustic branches of phonons mainly affect the thermal conductivity, one can only focus on the change of the acoustic PDOS. It can be noticed from Fig. 6(b) that the high-frequency PDOS of the strain of 8% is higher than the free of

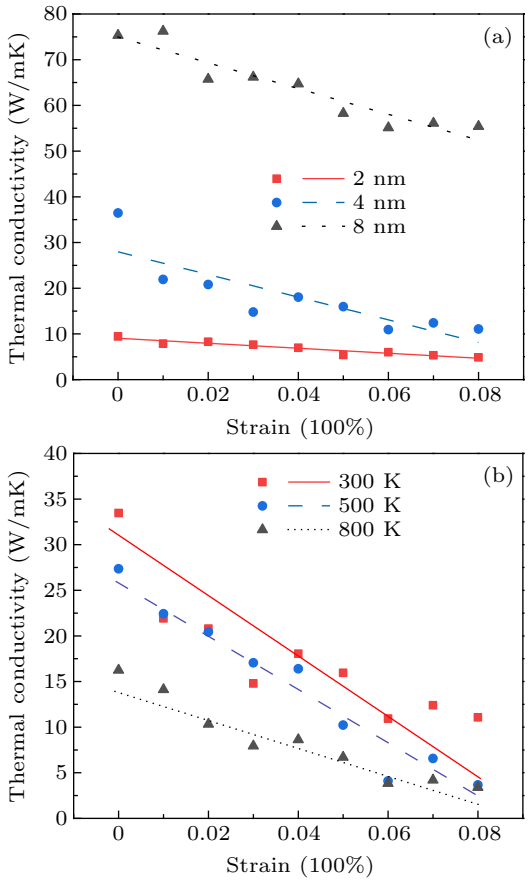


Fig. 5. The thermal conductivity of GaN nanofilms varies (a) with tensile strain for different thickness at 300 K, and (b) for different temperature with the thickness of 4 nm.

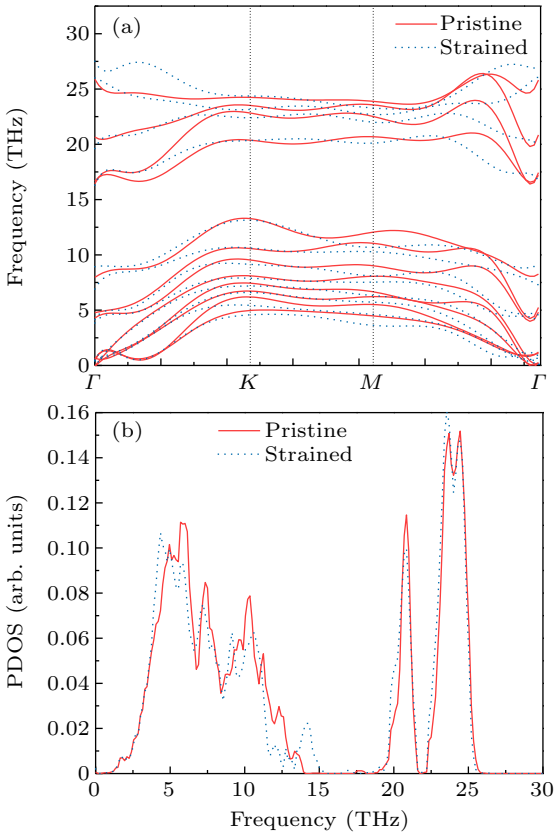


Fig. 6. Phonon dispersion (a) and phonon density of states (b) of 4 nm-GaN nanofilms with and without strain of 8% at 300 K.

strain, leading to the thermal conductivity even lower with the presence of the strain. From Fig. 6(a), the overall phonon dispersion curve of the strained GaN film is much smoother and less undulating, indicating smaller group velocity and lower thermal conductivity.

4. Summary

The dependence of the temperature, geometrical size, and strain field on the thermal conductivity of GaN nanofilms is investigated comprehensively through MD simulations. The simulation results demonstrate that the thermal conductivity of GaN nanofilms decreases with increasing temperature in the temperature range of 200 K–1000 K, the variation of thermal conductivity with the temperature becomes less sensitive for the thinner film. The smaller thickness of nanofilms and the larger tensile strain enable to decrease the thermal conductivity of GaN nanofilms. The size and strain effects of thermal conductivity are also sensitive to the temperature. The phonon properties of GaN nanofilms with various thickness and strain fields are calculated to explain the effects of thickness and strain fields on the thermal properties. The above findings could be helpful for optimizing the thermal performance of GaN-based HEMT devices through controlling the temperature, geometrical size and strain fields in GaN-based thin films.

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