Electron-Phonon Coupling and Thermal Transport Properties of GaN/AlGaN Heterojunction under Strain Regulation

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S1. MHHIM model

The Maximum Transport Model (MTM) [1] is an improvement of the acoustic mismatch model, which follows the same fine equilibrium and pure diffusive scattering, but is not limited to elastic scattering. In addition to the MTM model, another way to consider inelastic scattering at interfaces is to extend the fine balance principle to multiphonon processes, which is the basic idea of the Higher Harmonic Inelastic Model (HHIM) [2]. The three-phonon process consists of a process in which a phonon with the frequency $\omega 1$ splits into two phonons with the frequencies $\omega 2$ and $\omega 3$, i.e., $\omega 1=\omega 2+\omega 3$. The three-phonon process has a transmission coefficient and interfacial thermal conductance are shown in Eq. (1) and (2) below, respectively:

$$\alpha_1^{\mathrm{HHIM}}=\frac{\mathrm{h}2\omega\sum_p\left(v_2(2\omega,p)D_2(2\omega,p)\right)f(2\omega)}{2\mathrm{h}\omega\sum_p\left(v_1(\omega,p)D_1(\omega,p)\right)f(\omega)+\mathrm{h}2\omega\sum_p\left(v_2(2\omega,p)D_2(2\omega,p)\right)f(2\omega)} \tag{1}$$

$$h^3=\frac{1}{8}\int_0^{\omega_{\max}}\mathrm{h}\omega\sum_p\left(v_1(\omega,p)D_1(\omega,p)\right)\frac{\partial f(\omega)}{\partial T}\alpha_1^{\mathrm{HHIM}}\beta_1\mathrm{d}\omega \tag{2}$$

The HHIM, while based on the Diffusion Mismatch Model (DMM) [3] and considering the three-phonon interface process, only accounts for the process where two low-frequency phonons combine to produce a high-frequency phonon and does not consider the splitting process where a high-frequency phonon divides into two low-frequency phonons. The Modified High-Order Harmonic Interaction Model (MHHIM) [4] takes into account both of these interface processes, thereby addressing the limitations of the HHIM. This approach divides the phonons that do not participate in the two-phonon process into two parts: those that may participate in the merging process and those that may participate in the splitting process. The phonon energy emitted from the interface towards the GaN side consists of energy reflected back by the three-phonon process, energy transmitted by the two-phonon process, and energy transmitted by the three-phonon process. Eq. (3) provides the proportion of phonons on the GaN side that participate in the merging process.

$$\beta_{\mathrm{merge,GaN}}(\omega)=\frac{\alpha_{\mathrm{merge,GaN}}(\omega)}{\alpha_{\mathrm{merge,GaN}}(\omega)+\alpha_{\mathrm{split,GaN}}(\omega)} \tag{3}$$

where $\alpha_{\mathrm{merge,GaN}}$ denotes the transmission coefficient of the merging process in the three-phonon process on the GaN side. $\alpha_{\mathrm{split,GaN}}$ denotes the transmission coefficient of the splitting process. The modified

transmission coefficient of the merging process on the GaN side is shown in Eq. (4) below. The transmission coefficients of the other processes can be calculated in a similar way, and the total transmission coefficient can be expressed in Eq. (5). The modified interfacial thermal conductivity can be obtained by replacing the transmission coefficient in Eq. (5) with the total transmission coefficient in Eq. (2).

$$\alpha'_{\text{merge,GaN}}(\omega)=\frac{\hbar 2\omega\sum_{p}\left(v_2(2\omega,p)D_2(2\omega,p)\right)f(2\omega)\left(1-\alpha_2(\omega)\right)\beta_{\text{merge,AlGaN}}(2\omega)}{\left(\begin{array}{l}2\hbar\omega\sum_{p}\left(v_1(\omega,p)D_1(\omega,p)\right)f(\omega)\left(1-\alpha_1(\omega)\right)\beta_{\text{merge,GaN}}(\omega)+\\ \hbar 2\omega\sum_{p}\left(v_2(2\omega,p)D_2(2\omega,p)\right)f(2\omega)\left(1-\alpha_2(2\omega)\right)\beta_{\text{merge,AlGaN}}(2\omega)\end{array}\right)} \tag{4}$$

$$\alpha_1^{\text{MHHIM}}=\beta_{\text{merge,GaN}}\bullet\alpha'_{\text{merge,GaN}}+\beta_{\text{split,GaN}}\bullet\alpha'_{\text{split,GaN}} \tag{5}$$

Under steady state and relaxation time approximation, the BTE can be simplified as:

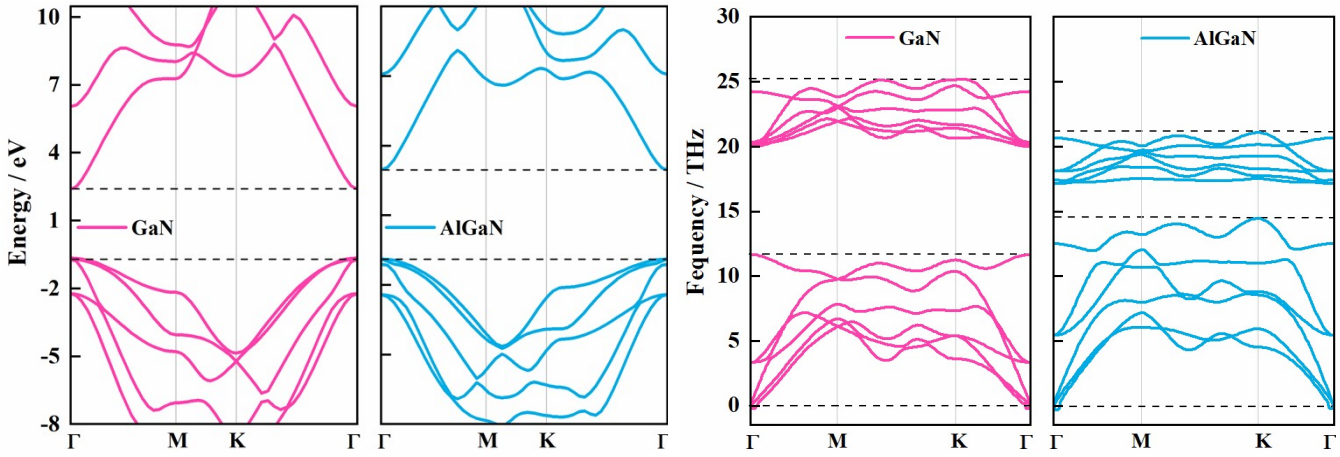
$$\nabla\cdot\left(v_g s e''\right)=\frac{e^0-e''}{\tau} \tag{6}$$

$$e''=1/4\pi\int_{\Delta\omega}\hbar\omega D(\omega)\left(f-f_{\text{ref}}\right)d\omega \tag{7}$$

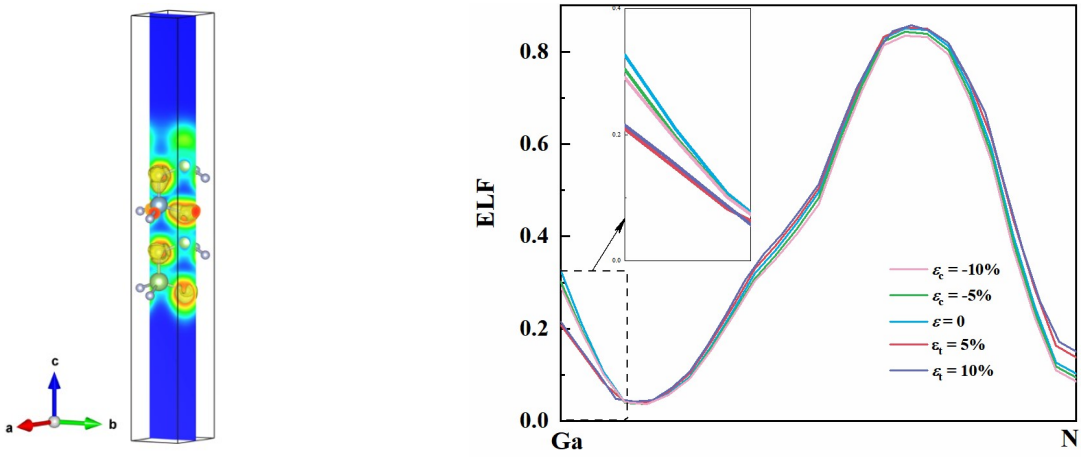
where e" denotes the nonequilibrium phonon energy density, e^0 denotes the equilibrium phonon energy density, f is the nonequilibrium phonon distribution function; f_{ref} is the phonon equilibrium distribution function at the ambient temperature (300 K); D is the phonon density of state, v_g is the group velocity of the phonon, τ is the relaxation time of the phonon, $\hbar$ is the approximate Prandtl number, s is the unit direction vector; ω is the phonon frequency. Integrating Eq. (7) over the entire cubic angle space and frequency space yields an expression for the heat flow density:

$$q=\sum_{p}\int_{\omega_{\min,p}}^{\omega_{\max,p}}\int_{4\pi}v e d\Omega d\omega \tag{8}$$

where $\omega_{\max,p}$ and $\omega_{\min,p}$ denote the upper and lower frequency limits for a given phonon branch "p", respectively.



(a) (b)



(c) (d)

Fig. S1 (a) Electronic energy band structure and (b) dispersion curves of GaN and AlGaN in the free state, (c) three-dimensional versus two-dimensional bonded cross-section of the ELF of the heterojunction in the initial state, and (d) variation of the ELF from Ga to N atoms with strain intensity

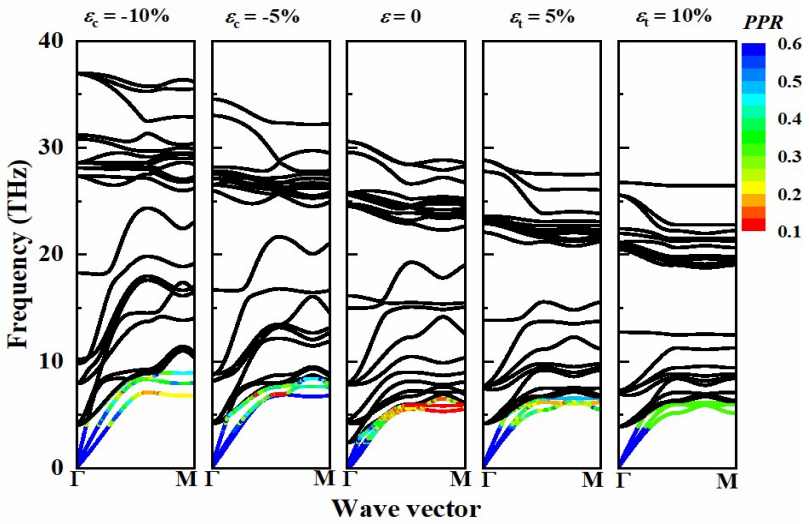


Fig. S2 Variation of phonon dispersion with strain for heterogeneous junctions of projected PPR.

References

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