Supplementary material for

Nonequilibrium electron-phonon coupling across the interfaces between Al nanofilm and GaN

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In this work, all calculations based on density functional theory (DFT) are implemented through the Vienna ab-initio simulation package (VASP) [1]. The interaction between electrons and ions is described by the PAW method, and the exchange correlation functional is described by the Perdew-Burke-Ernzerhof (PBE) form in the generalized gradient approximation (GGA) [2, 3]. The plane wave cutoff energy of the calculated structures is set to 450 eV. The 4×4×4 Monkhorst-Pack k-points grid in first Brillouin zone is used to ensure accurate calculations. The structures are fully relaxed until the convergence standard of energy differences reach the 10^{-6} eV and the force reaches the 10^{-4} eV/Å. The finite displacement method is used to calculate the second-order interatomic force constants (IFCs) and based on a 4×4×4 supercell with 4×4×4 k-points mesh. The 2nd IFCs are extracted by PHONOPY package [4]. The calculated phonon dispersion, phonon density of states and phonon group velocities are shown in Fig. S1 (a), (b)&(c). To determine the phonon-phonon coupling factors, the mode heat capacity and scattering rate in the full Brillouin zone are calculated through ShengBTE package [5]. The anharmonic IFCs are extracted by a series of supercells containing irreducible atomic displacement information generated by the thirdorder.py script, in which the interaction between atoms is cutoff up to the sixth rest neighbor. The calculated heat capacity and scattering rate are shown in Fig. S1 (d)&(e). The ensemble-averaged scattering rate can be obtained through the following equations.

$$\overline{\Gamma}_i = \frac{\sum C(\omega)\Gamma_i(\omega)}{\sum C(\omega)} \tag{1}$$

where i represents the phonon modes. $C(\omega)$ is the mode heat specific, and $\Gamma_i(\omega)$ is the scattering rate of mode i. The phonon lifetime can be obtained after obtaining the ensemble-averaged scattering rate.
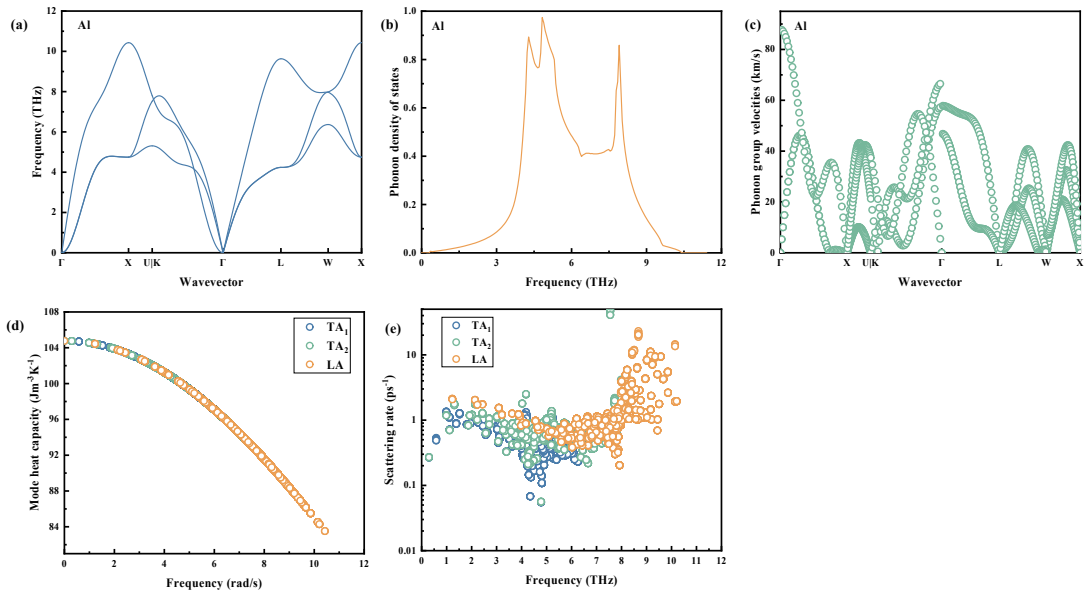
Fig. S1 (a) Phonon dispersion, (b) phonon density of states, (c) phonon group velocities, (d) mode heat capacity in full Brillouin zone and (e) scattering rate in full Brillouin zone

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