Electronic Supplementary Material (ESI) for Nanoscale Horizons.

Supporting Information

Mechanical Regulation to Interfacial Thermal Transport in GaN/Diamond Heterostructures for Thermal Switch

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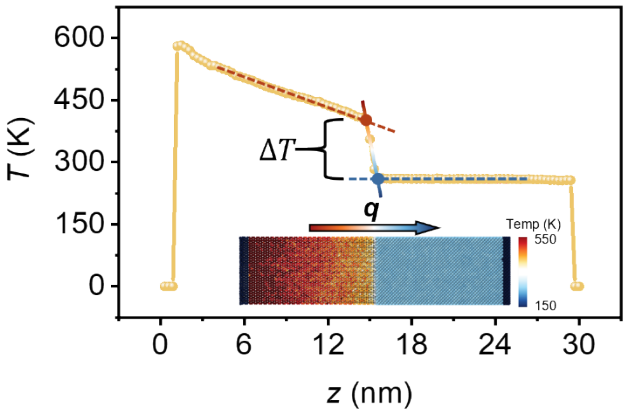

Figure S1. Temperature profile for the interface thermal boundary conductance calculation ($\varepsilon = 0\%$). The illustration shows the temperature distribution of atoms. The heat flux direction is from GaN to diamond. Three curves are obtained by sequentially fitting temperature profiles of GaN, heterostructure interface, and diamond. Then, the intersection points of these three curves are determined, yielding two points. These two points represent the maximum and minimum temperatures at the interface, with the temperature difference between them defining the temperature drop ΔT across the interface.

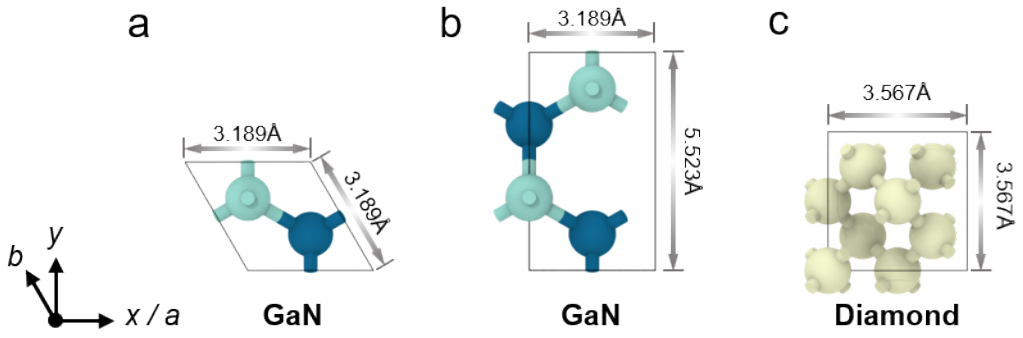

Figure S2. The crystal cell configuration and lattice constants of (a) GaN (wurtzite crystal structure), (b) an orthogonalization of the GaN wurtzite crystal structure, and (c) diamond (diamond cubic lattice structure).

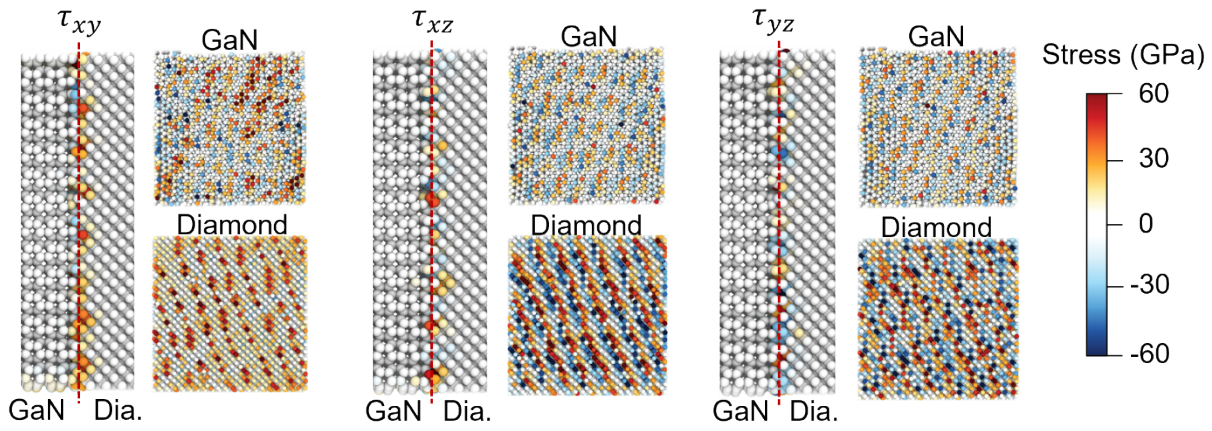

Figure S3. The planar distribution of stress τ_{xy}, τ_{xz} and τ_{yz}in both *y*-*z* and *x*-*y* planes at the interface without nominal strain.

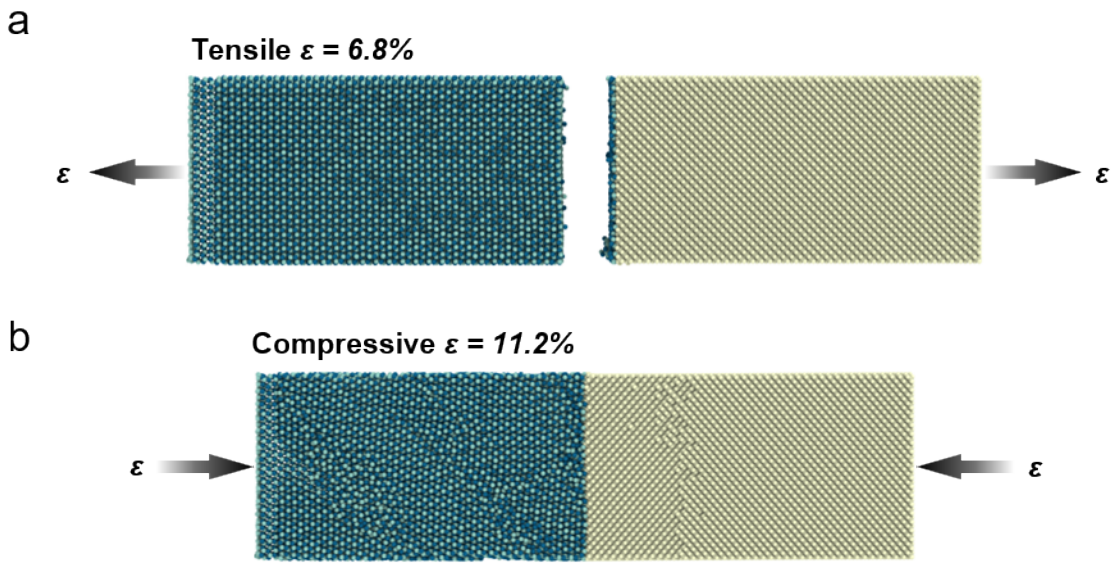

Figure S4. The snapshots of the failure and crushing behavior at the interface of the heterostructure. (a) Tensile strain-induced failure. (b) Compressive strain-induced crushing.

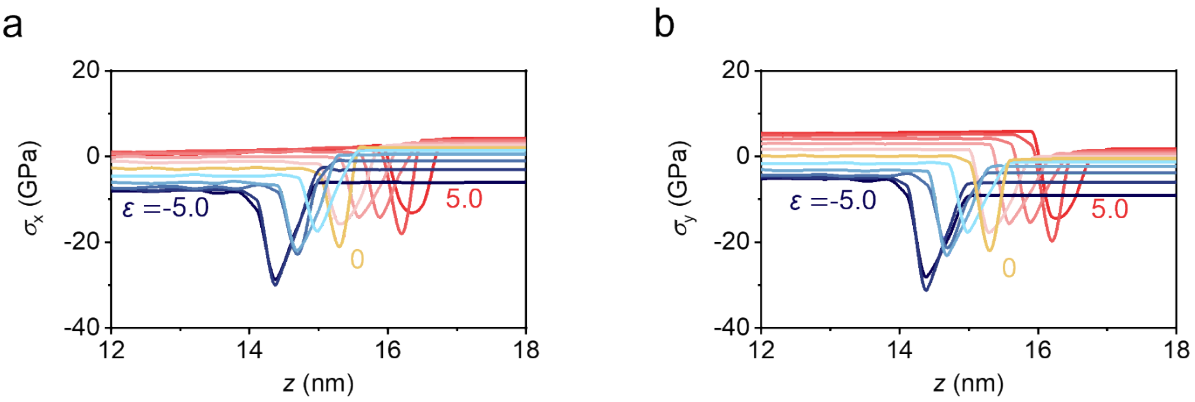

Figure S5. The distribution of (a) σ_x, and (b) σ_y along the z-direction in the GaN/diamond heterostructures under different mechanical loading.

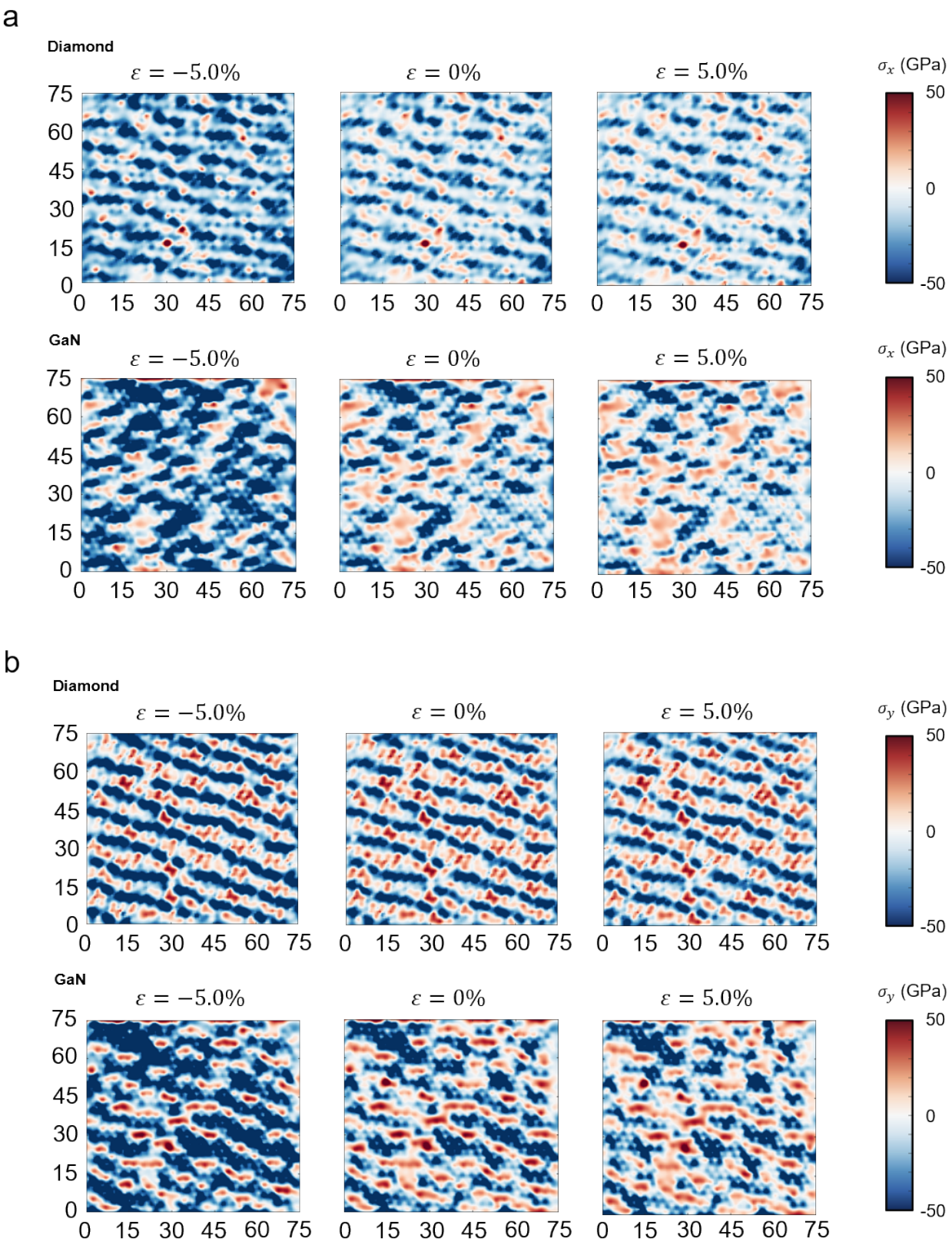

Figure S6. The planar distribution of (a) σ_x, and (b) σ_y in the *x*-*y* plane at the interface with various

nominal strain of 0, -5%, and 5%.

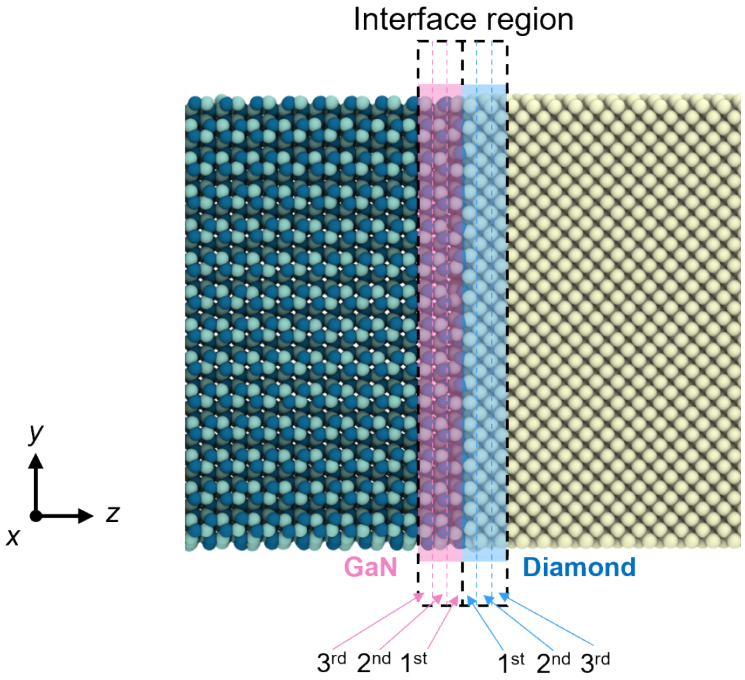

Figure S7. Layering scheme of the interface region. According to the range of stress along the *z*-coordinate (interface region), the diamond and GaN atoms at the interface are divided into three layers uniformly along the *z*-direction. The 1st layer is the direct contact layer between diamond and GaN at the interface, which produces the highest stress, while the 2nd and 3rd layers are also the stress-affected areas near the interface.

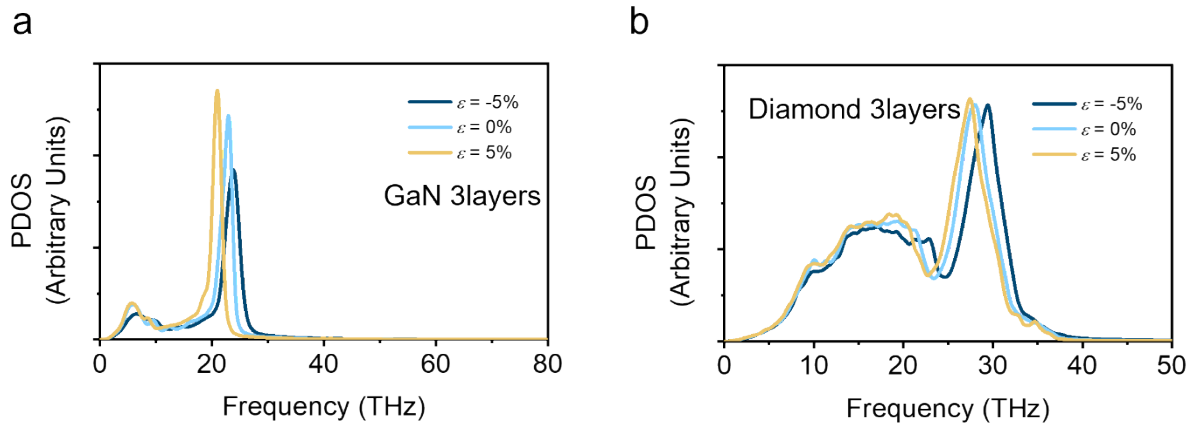

Figure S8. The PDOS of (a) GaN, and (b) diamond in the stress variation region (comprising three layers) at the interface.