Supplementary Information

Deep-potential driven multiscale simulation of gallium nitride devices on boron arsenide cooling substrates

Jing Wu†, E Zhou†, An Huang†, Hongbin Zhang, Ming Hu, and Guangzhao Qin†,4,5,*

†State Key Laboratory of Advanced Design and Manufacturing Technology for Vehicle, College of Mechanical and Vehicle Engineering, Hunan University, Changsha 410082, P. R. China
‡Institut für Materialwissenschaft, Technische Universität Darmstadt, Darmstadt, 64289, Germany
§Department of Mechanical Engineering, University of South Carolina, Columbia, SC 29208, USA
‡†Research Institute of Hunan University in Chongqing, Chongqing 511300, Guangdong Province, China
‡‡Greater Bay Area Institute for Innovation, Hunan University, Guangzhou 511300, Guangdong Province, China
‡‡†Key Laboratory of Computational Physical Sciences (Fudan University), Ministry of Education
‡‡‡Present address: School of Energy and Power Engineering, Huazhong University of Science and Technology, Wuhan, Hubei 430074, China

* Author to whom all correspondence should be addressed. E-Mail: gzqin@hnu.edu.cn
Supplementary Figure 1 The comparison of group velocity, phonon relaxation time, scattering phase space, and Grüneisen parameter between BAs and GaN.
Supplementary Figure 2 The visualization of phonon eigenvectors for GaN-BAs interface at different frequencies. The color bar represents the amplitude of the normalized eigenvectors and the arrow represents the magnitude and direction of the amplitude.
Supplementary Figure 3 (a) GaN-BAs heterostructures after relaxation and (b) the atomic energy distribution. The color bar represents the magnitude of atomic energy.
**Supplementary Figure 4** Force distribution in GaN-BAs heterostructures. (a) GaN-BAs heterostructure after relaxation. (b) Force $f_x$ in the $x$-direction of GaN-BAs; (c) Force $f_y$ in the $y$-direction of GaN-BAs; (d) Force $f_z$ in the $z$-direction of GaN-BAs. The color bar represents the magnitude of atomic force.
Supplementary Figure 5 Stress distribution in GaN-BAs heterostructures. (a) GaN-BAs heterostructure after relaxation. (b) Stress $\sigma_x$ in the $x$-direction of GaN-BAs; (c) Stress $\sigma_y$ in the $y$-direction of GaN-BAs; (d) Stress $\sigma_z$ in the $z$-direction of GaN-BAs. The color bar represents the magnitude of atomic stress.
Supplementary Figure 6 The temperature-dependent spectral heat flux and phonon transmission coefficient in GaN-BAs heterostructures.
Supplementary Figure 7 The length-dependent ITC in GaN-BAs heterostructures.
**Supplementary Figure 8** The length-dependent thermal conductivity of GaN and BAs.
**Supplementary Table. 1** The percentage contribution of $\kappa$ from the two transverse-acoustic (TA$_1$ and TA$_2$), longitudinal-acoustic (LA) and optical branches.

|          | GaN-inplane | GaN-outplane | BAs-in/outplane |
|----------|-------------|--------------|-----------------|
| TA$_1$   | 21.2        | 19.7         | 26.4            |
| TA$_2$   | 23.4        | 27.6         | 45.1            |
| LA       | 24.7        | 21.1         | 28.4            |
| Optical  | 30.7        | 31.6         | 0.1             |