Electronic Supplementary Information

# Significant enhancement of lattice thermal conductivity of monolayer AlN under bi-axial strain: A first principles study

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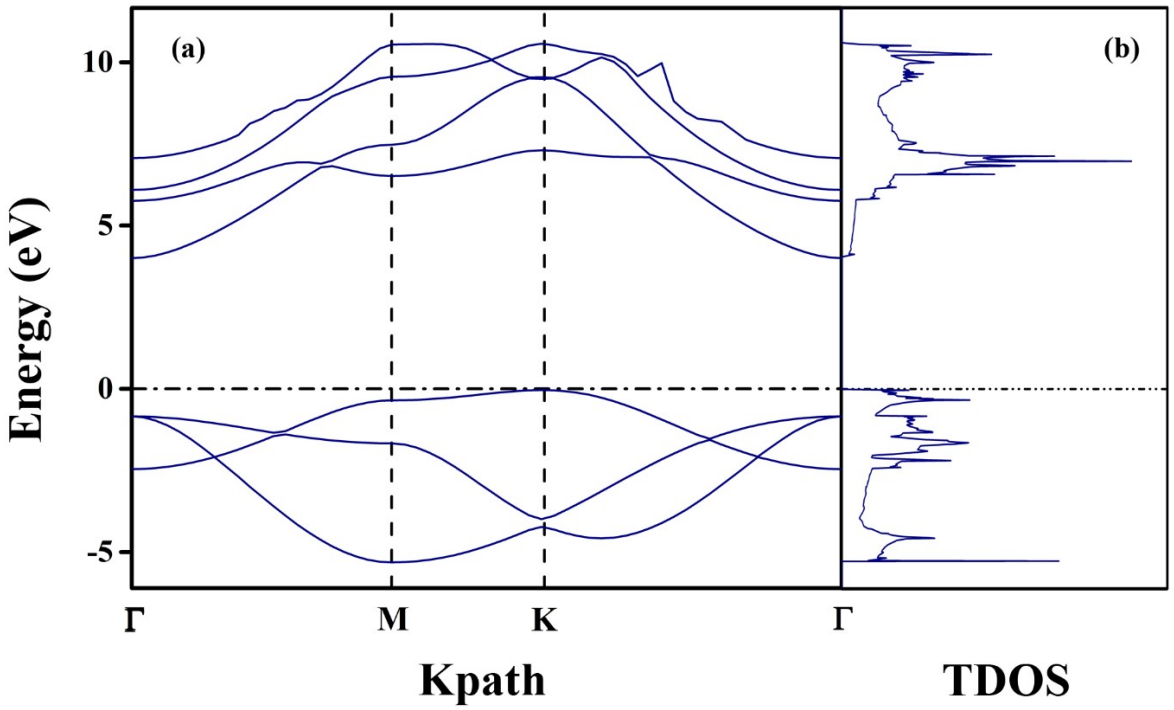


Figure 1S. a) Electronic band structure of pristine monolayer AlN, b) The total density of states (TDOS) of monolayer AlN

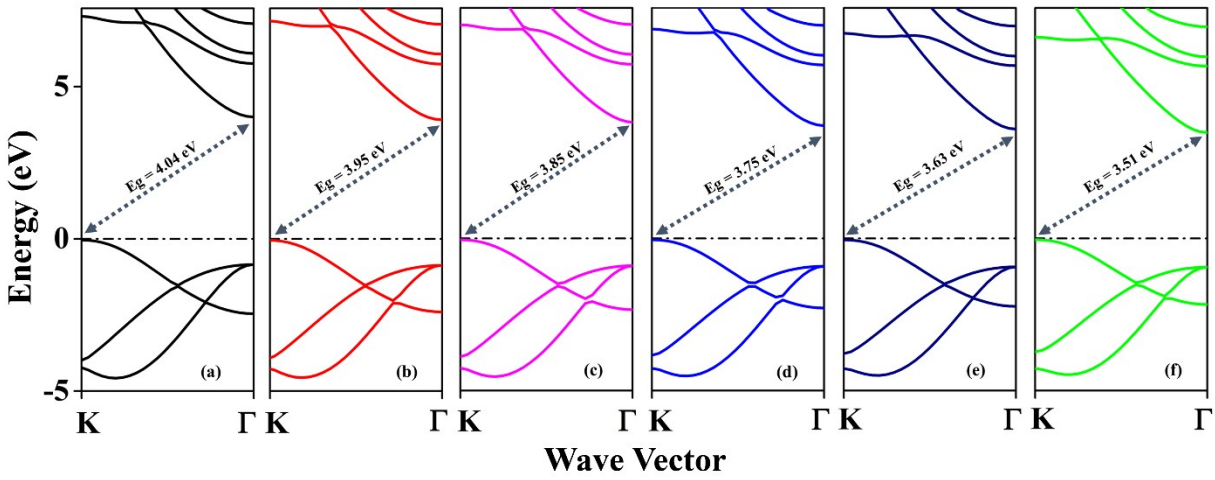


Figure 2S. Change in band gap of monolayer AlN with introduction of bi-axial strain a) Pristine, b) 1 %, c) 2 %, d) 3 %, e) 4 % and f) 5 %

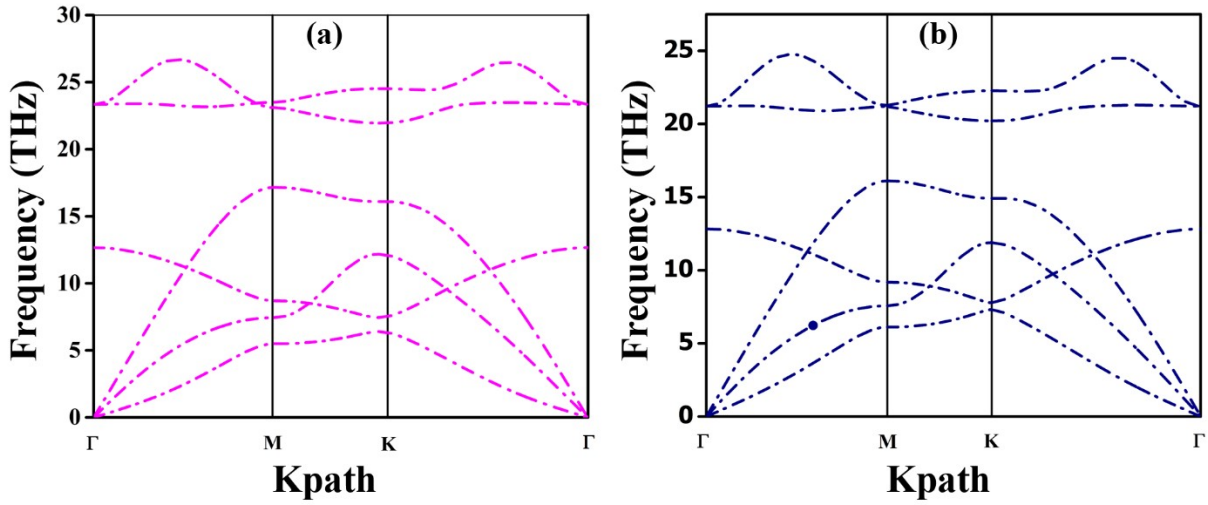


Figure 3S. Phonon dispersions of strained structures of monolayer AlN with applied strain a) 2 % and b) 4 %

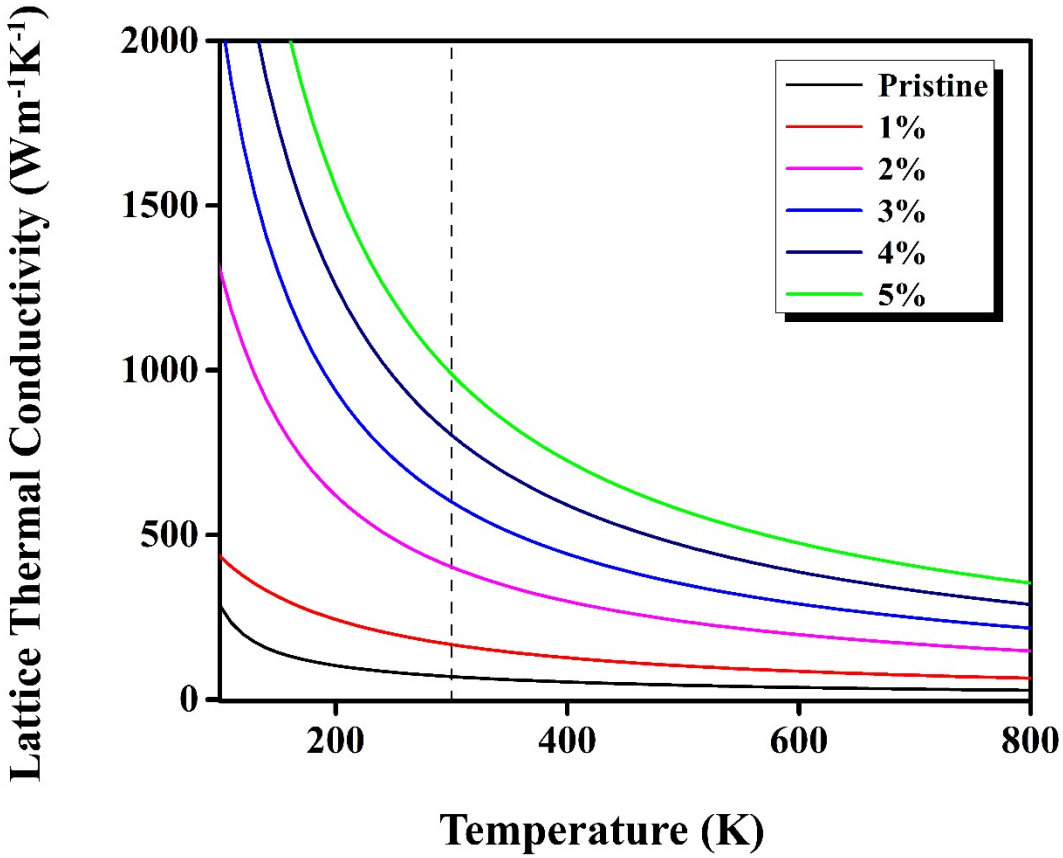


Figure 4S. Lattice thermal conductivity variation with temperature for pristine and different strained structures (1 % - 5 %) by relaxation time approximation (RTA) method

Table 1S. Values of lattice thermal conductivity of unstrained and strained monolayer AlN calculated by relaxation time approximation (RTA) method at 300 K.

| **Applied bi-axial strain (in %)** | **Lattice thermal conductivity ($W\ m^{-1}\ K^{-1}$)** |
|---|---|
| Pristine | 69.54 |
| 1 % | 166.83 |
| 2 % | 402.31 |
| 3 % | 600.13 |
| 4 % | 802.85 |
| 5 % | 988.29 |

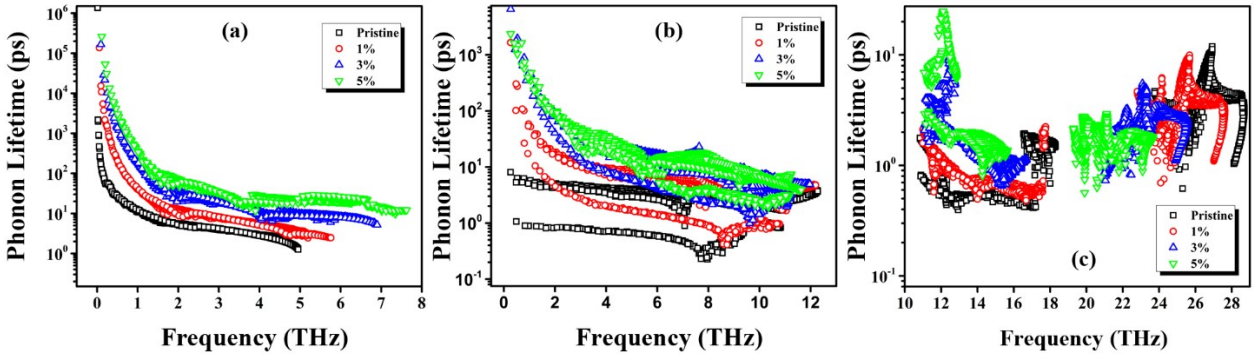


Figure 5S. Phonon lifetime of different phonon modes for pristine and strained structures (1 %, 3 % and 5 %), a) ZA mode, b) TA modes and c) LA modes

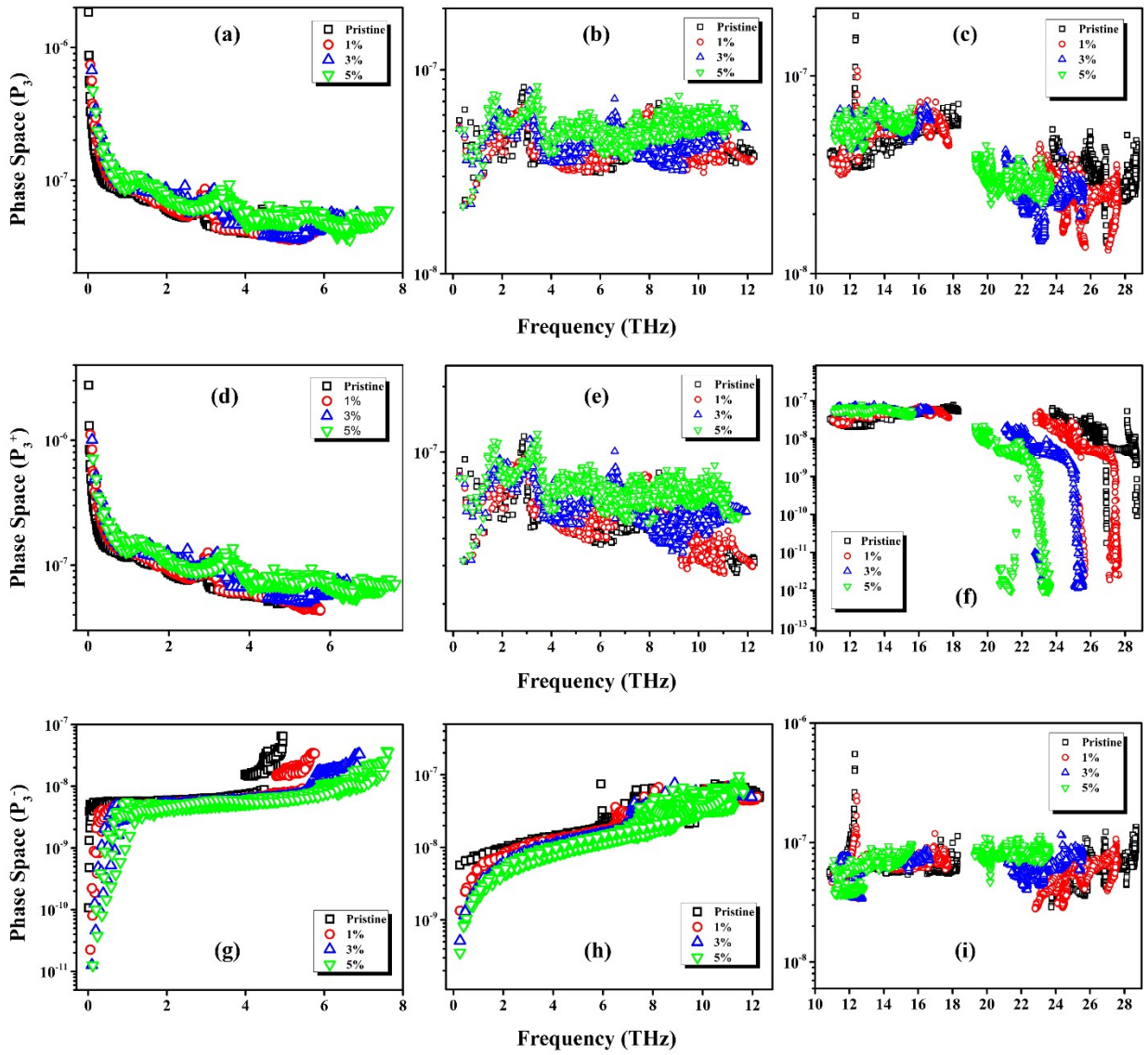


Figure 6S. Three-phonon scattering phase space of different phonon modes for pristine and strained structures (1 %, 3 % and 5 %), the total anharmonic three-phonon scattering phase space ($P_3$) for a) ZA mode, b) LA and TA modes, c) Optical modes, anharmonic three-phonon scattering phase space of absorption process ($P_3^+$) for d) ZA mode, e) LA and TA modes, f) Optical modes, and anharmonic three-phonon scattering phase space of emission process ($P_3^-$) for a) ZA mode, b) LA and TA modes, c) Optical modes

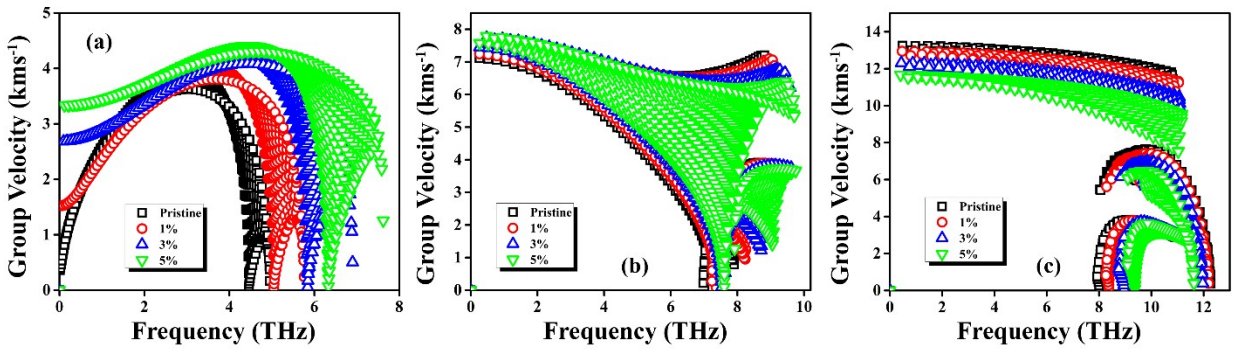


Figure 7S. Mode resolved phonon group velocities for pristine and strained structures (1 %, 3 % and 5 %), a) ZA mode, b) TA modes and c) LA modes

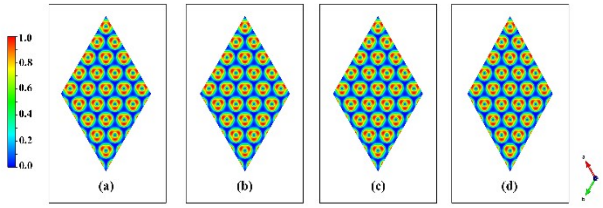


Figure 8S. Top view of electron localization function (ELF) of monolayer AlN for unstrained and strained structures a) pristine, b) 1 % strain, c) 3 % strain and d) 5 % strain

Table 2S. Born effective charges (Z*) of Al and N atoms and the dielectric constants (ε) of unstrained and strained monolayer AlN

| Strain (in %) | Direction | Z*(Al) | Z*(N) | ε |
|---|---|---|---|---|
| Pristine | xx | 2.713428 | -2.713428 | 1.570914 |
| | xy | 0.000000 | 0.000000 | 0.000000 |
| | xz | 0.000000 | 0.000000 | 0.000000 |
| | yx | 0.000000 | 0.000000 | 0.000000 |
| | yy | 2.713428 | -2.713428 | 1.570914 |
| | yz | 0.000000 | 0.000000 | 0.000000 |
| | zx | 0.000000 | 0.000000 | 0.000000 |
| | zy | 0.000000 | 0.000000 | 0.000000 |
| | zz | 0.404667 | -0.404667 | 1.157815 |
| 1 % | xx | 2.727884 | -2.727884 | 1.587260 |
| | xy | 0.000000 | 0.000000 | 0.000000 |
| | xz | 0.000000 | 0.000000 | 0.000000 |
| | yx | 0.000000 | 0.000000 | 0.000000 |
| | yy | 2.727884 | -2.727884 | 1.587260 |
| | yz | 0.000000 | 0.000000 | 0.000000 |
| | zx | 0.000000 | 0.000000 | 0.000000 |
| | zy | 0.000000 | 0.000000 | 0.000000 |
| | zz | 0.400569 | -0.400569 | 1.158288 |
| 2 % | xx | 2.742100 | -2.742100 | 1.604816 |
| | xy | 0.000000 | 0.000000 | 0.000000 |
| | xz | 0.000000 | 0.000000 | 0.000000 |
| | yx | 0.000000 | 0.000000 | 0.000000 |
| | yy | 2.742100 | -2.742100 | 1.604816 |
| | yz | 0.000000 | 0.000000 | 0.000000 |
| | zx | 0.000000 | 0.000000 | 0.000000 |
| | zy | 0.000000 | 0.000000 | 0.000000 |
| | zz | 0.396331 | -0.396331 | 1.158754 |
| 3 % | xx | 2.756099 | -2.756099 | 1.623683 |
| | xy | 0.000000 | 0.000000 | 0.000000 |
| | xz | 0.000000 | 0.000000 | 0.000000 |
| | yx | 0.000000 | 0.000000 | 0.000000 |
| | yy | 2.756099 | -2.756099 | 1.623683 |
| | yz | 0.000000 | 0.000000 | 0.000000 |
| | zx | 0.000000 | 0.000000 | 0.000000 |
| | zy | 0.000000 | 0.000000 | 0.000000 |
| | zz | 0.391850 | -0.391850 | 1.159212 |
| 4 % | xx | 2.769843 | -2.769843 | 1.643942 |
| | xy | 0.000000 | 0.000000 | 0.000000 |
| | xz | 0.000000 | 0.000000 | 0.000000 |
| | yx | 0.000000 | 0.000000 | 0.000000 |
| | yy | 2.769843 | -2.769843 | 1.643942 |

| | | | | |
|---|---|---|---|---|
| | yz | 0.000000 | 0.000000 | 0.000000 |
| | zx | 0.000000 | 0.000000 | 0.000000 |
| | zy | 0.000000 | 0.000000 | 0.000000 |
| | zz | 0.387291 | -0.387291 | 1.159662 |
| 5 % | xx | 2.783439 | -2.783439 | 1.665895 |
| | xy | 0.000000 | 0.000000 | 0.000000 |
| | xz | 0.000000 | 0.000000 | 0.000000 |
| | yx | 0.000000 | 0.000000 | 0.000000 |
| | yy | 2.783439 | -2.783439 | 1.665895 |
| | yz | 0.000000 | 0.000000 | 0.000000 |
| | zx | 0.000000 | 0.000000 | 0.000000 |
| | zy | 0.000000 | 0.000000 | 0.000000 |
| | zz | 0.382481 | -0.382481 | 1.160104 |