Supporting Information

Lattice deformation and phase transition of aluminum nitride studied by density functional theory calculation

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S-1. Total energy in wurtzite-type AlN

In the main text, the variation of lattice parameters of wurtzite-type (WZ-type) phase under external uniaxial pressure is shown in Fig. 1, and Fig. 5(a) shows variation of enthalpy of the WZ-type phase under the external pressure as a function of a-axis lattice constant (a_0). Here, variation of total energy in AlN under uniaxial pressure is shown in Fig. S1 as a function of a_0 for comparison with Fig. 5(a). It is clearly indicated that total energy takes minima when AlN was free from strain and a_0 was converged at 3.1208 Å. That confirms that AlN with a_0=3.1208 and c_0= 4.9969 Å is the fully relaxed equilibrium values under present calculation conditions.

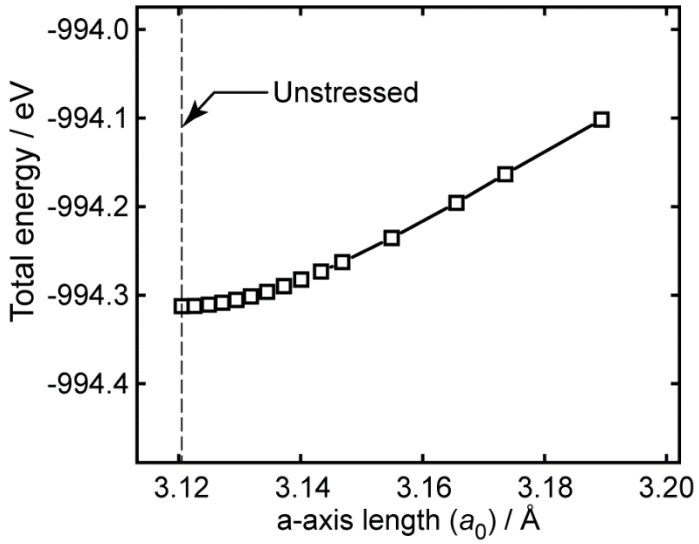

Figure S1 Total energy in AlN crystallized in wurtzite-form as a function of assumed a-axis length.