Supporting Information

Energy minimization was achieved through the conjugate gradient method during the structural relaxation process, ensuring the stability of the structure. We further investigated the thermodynamic stability of the two anti-phase boundaries at finite temperatures using ab initio molecular dynamics (AIMD) simulations. The AIMD simulation was carried out for 10 ps. The calculation adopted the density functional theory (DFT) quantum mechanics first-principles calculation method and is carried out by the Vienna Ab initio Simulation Package (VASP). The cutoff energy of the plane wave was 400 eV, and the energy convergence criterion was 10^{-4} eV/atom for electronic relaxation. Structural relaxation with a convergence criterion of all interatomic forces below 0.03 eV/Å. The Calculation results are shown in Fig. S1. The calculation results indicate that at different temperatures, the two types of anti-phase boundary models always exhibit stable thermodynamic stability.

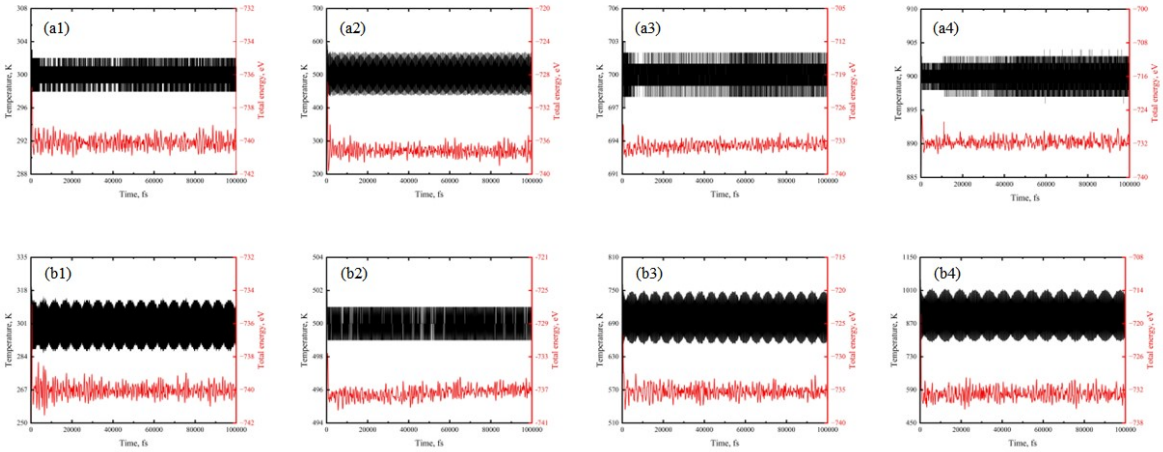

Fig. S1 Variation of the total energy and temperature as a function of time in AIMD simulation at 300 K, 500 K, 700 K, and 900 K, (a1)-(a4) APB_I; (b1)-(b4) APB_{II}.