Supporting information

Deformation Mechanisms in the High-Efficiency Thermoelectric Layered Zintl Compounds

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Deformation mechanisms of Mg_3Sb_2 along the (001)/<100> slip system

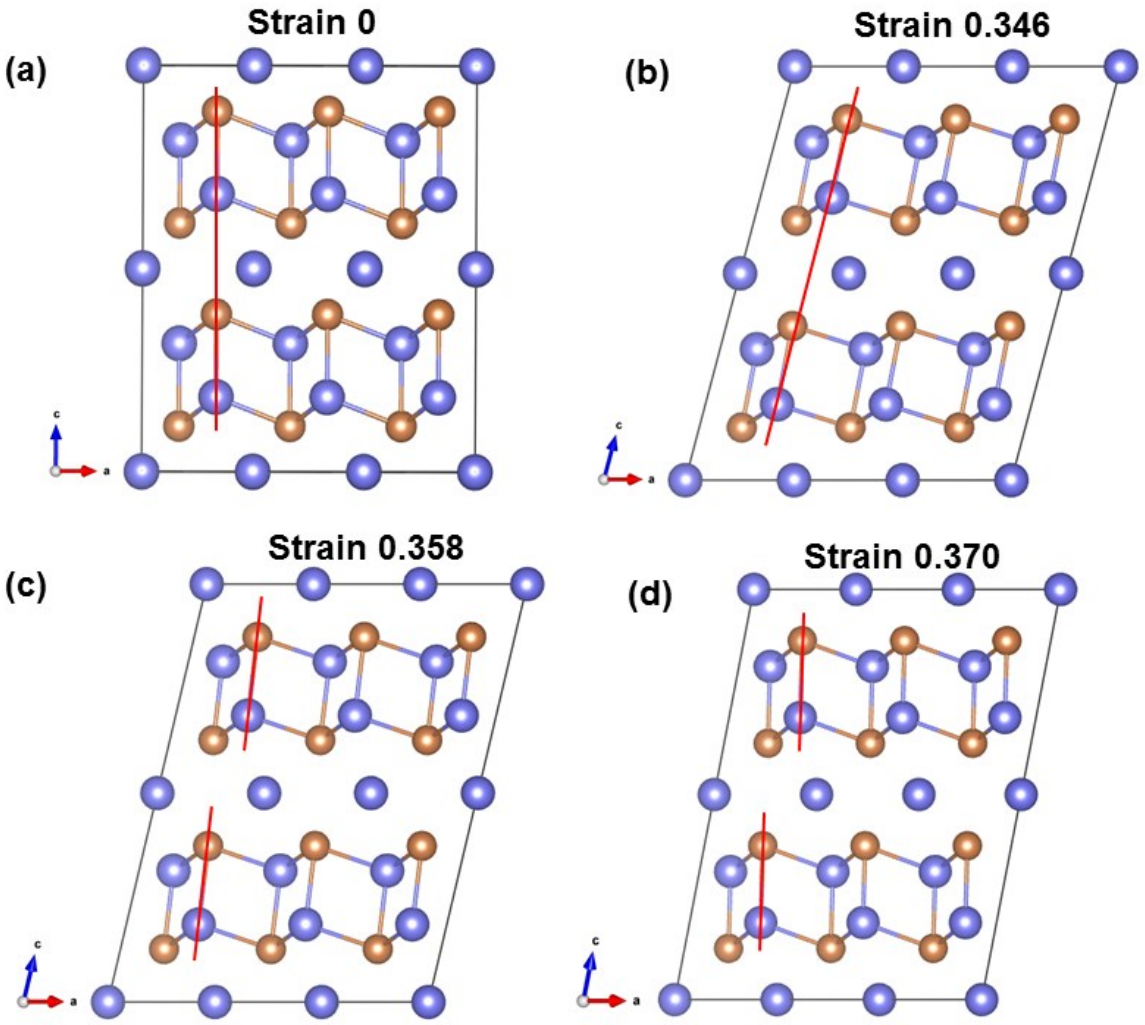

Figure S1. The atomic structures of Mg_3Sb_2 along the (001)/<100> slip system: (a) structure at strain 0 corresponding to the equilibrium condition, (b) structure 0.346 corresponding to the ideal strength, (c) structure at 0.358 strain before failure strain, (d) structure at failure strain of 0.370. The red lines displayed in Figure S1 show the slippage of layered $[Mg_2Sb_2]^{2-}$ substructures.

Deformation mechanisms of Mg_3Sb_2 along the (100)/<110> slip system

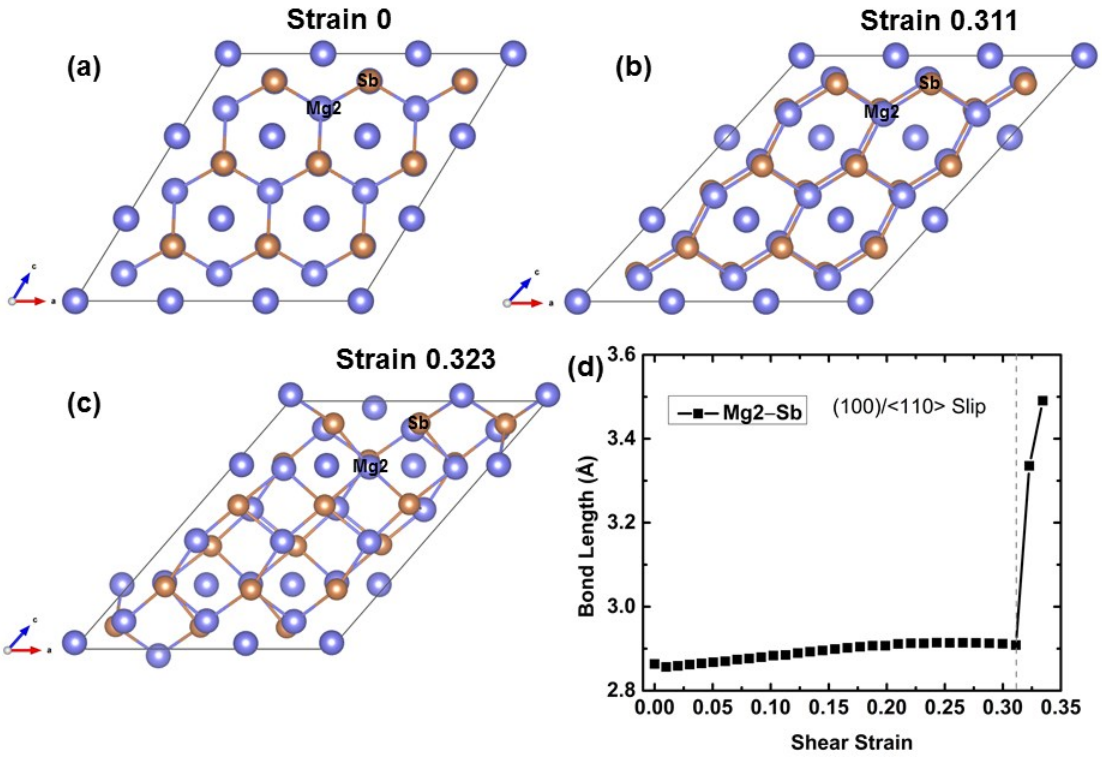

Figure S2. The atomic structures of Mg_3Sb_2 along the (100)/<110> slip system: (a) structure at strain 0 corresponding to the equilibrium condition, (b) structure at 0.311 strain before failure strain, (c) structure at failure strain of 0.323 corresponding to the critical point for bond breaking, (d) The average covalent Mg2–Sb bond length with the increasing shear strain along the (100)/<110> slip system. The gray dashed line in Figure S2(d) represents the strain just before failure.