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Supporting Information

Determining ideal strength and failure mechanism of thermoelectric $CuInTe_2$ from quantum mechanics

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Explanation on how we compute the stress-strain relations

To examine the mechanical response and failure mechanism of $CuInTe_2$, we applied pure shear and tensile deformation on it by imposing the shear or tensile strain on a particular supercell system while allowing structural relaxation along the other five strain components (Figure. S1). The biaxial shear deformation was also examined to mimic the stress conditions in Vickers indentation experiments (Figure. S1). Here we considered a biaxial stress distribution beneath an indenter with a shear stress (σ_{xz}) and a normal compressive stress component (σ_{zz}). They are constrained as $\sigma_{zz} = \sigma_{zz} \tan\phi$, where $\phi = 68^{\circ}$ is the centerline-to-face angle for a Vickers indenter.[1] The computed stress-strain relations are true stress-strain relations. The residual stresses for relaxation along the other strain components both in pure shear and biaxial shear deformations are all less than 0.2 GPa.

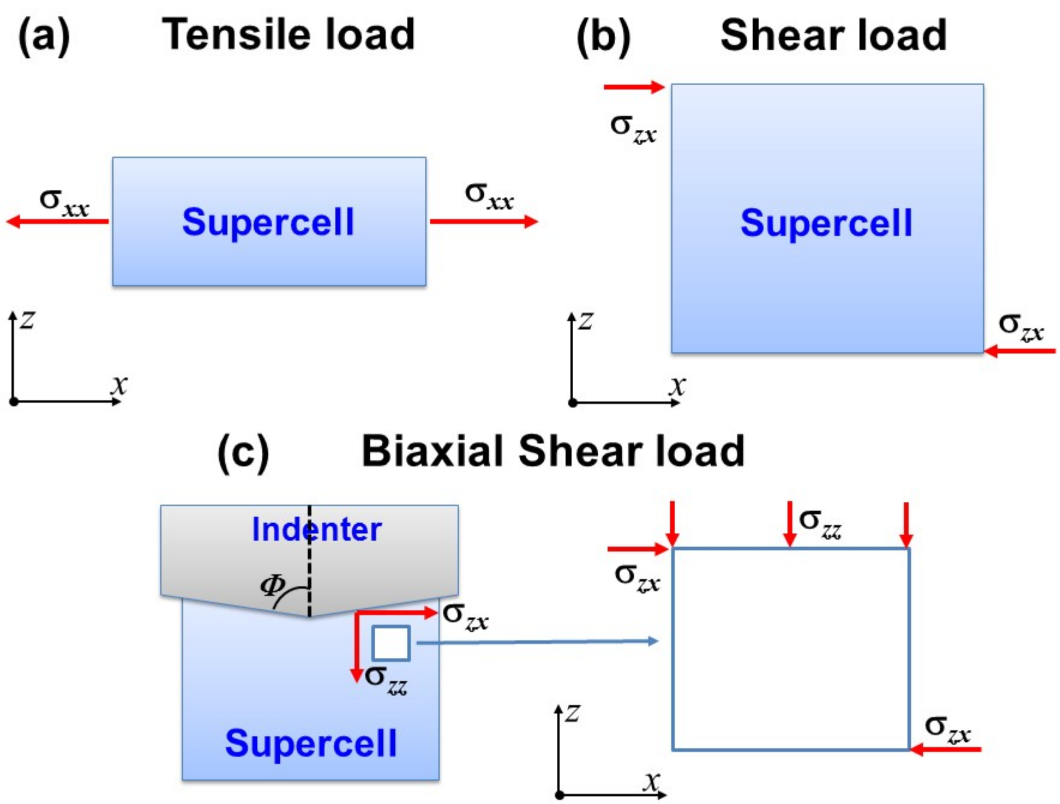

Figure S1. Sketch of (a) tensile load, (b) shear load, and (c) biaxial shear load.

The ELF change against shear strain for $CuInTe_2$ under (221)[11-1] pure shear load

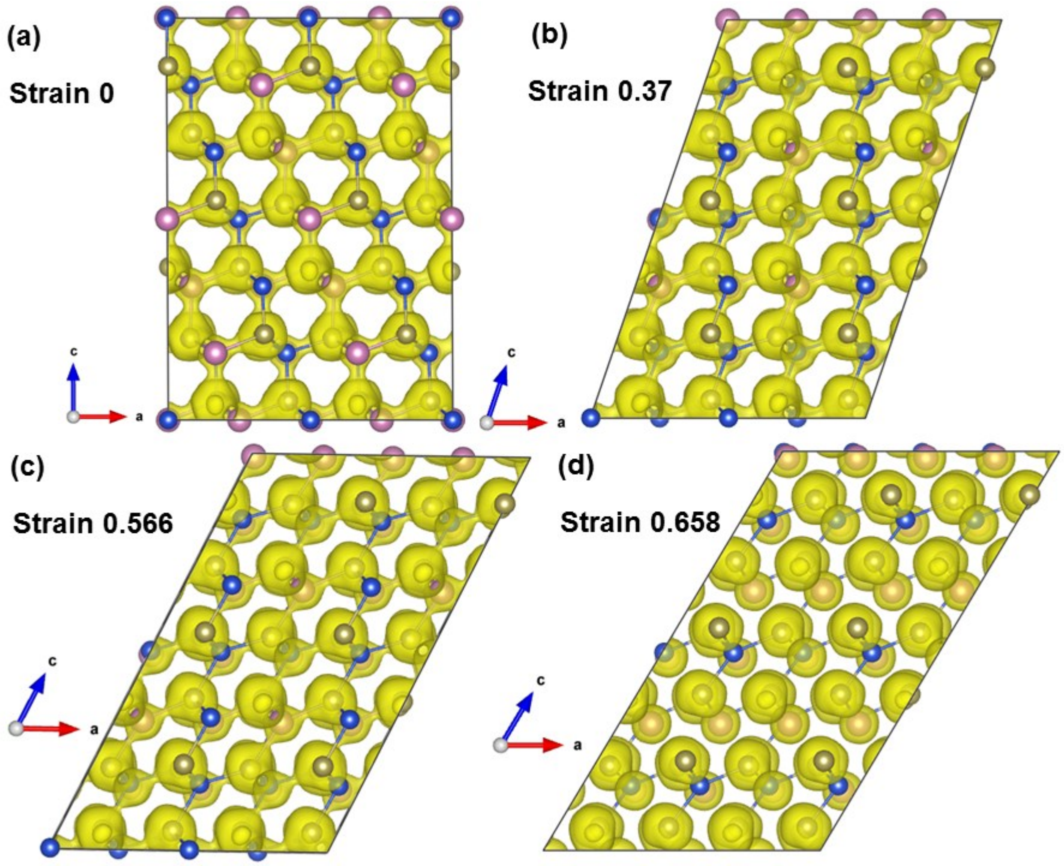

Figure S2. Calculated atomic configurations combined with isosurfaces of the electron localization function (ELF) for shear loads along the (221)[11-1] slip system: (a) shear strain 0 corresponds to the initial stage, (b) shear strain 0.37 corresponds to the ideal strength, (c) shear strain 0.566 before structural softening, and (d) shear strain 0.658 corresponding to the highly softened structure. The ELF is represented by the shallow yellow region.

The ELF change against uniaxial tensile strain for $CuInTe_2$ under [1-10] tension load

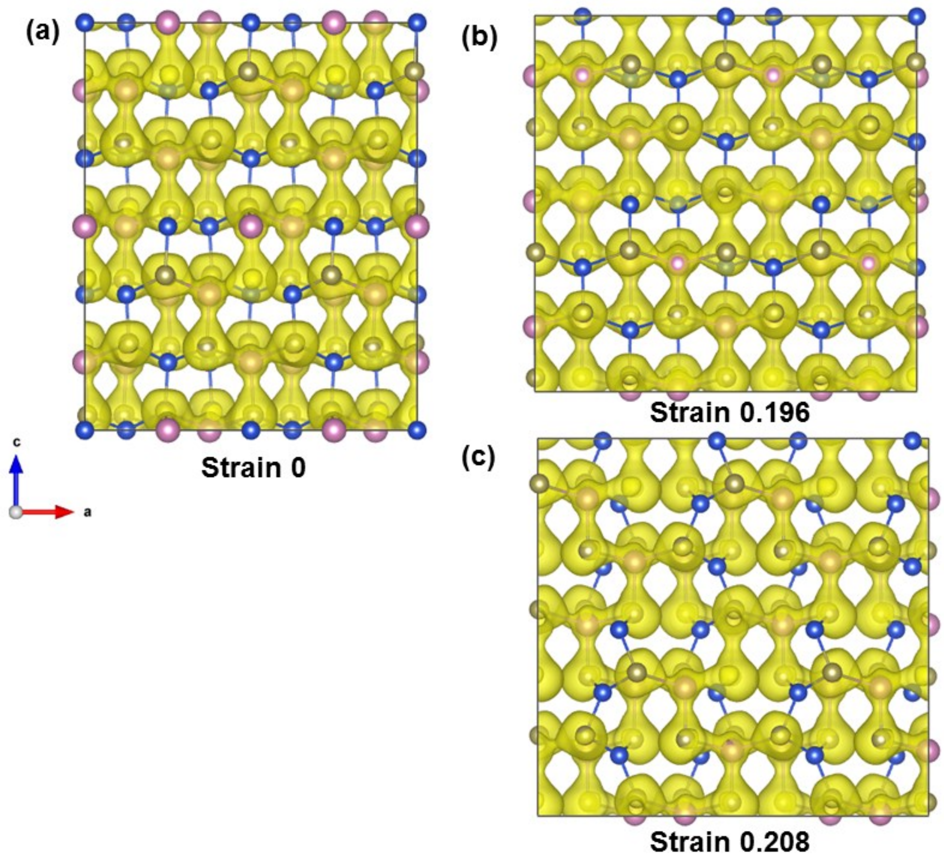

Figure S3. Calculated atomic configurations combined with isosurfaces of the electron localization function (ELF) for tensile loads along the [1-10] tensile system: (a) tensile strain 0 corresponds to the initial stage, (b) tensile strain 0.196 before failure, (c) failure strain 0.208. The ELF is represented by the shallow yellow region.

The ELF change against shear strain for $CuInTe_2$ under (221)[11-1] biaxial shear load

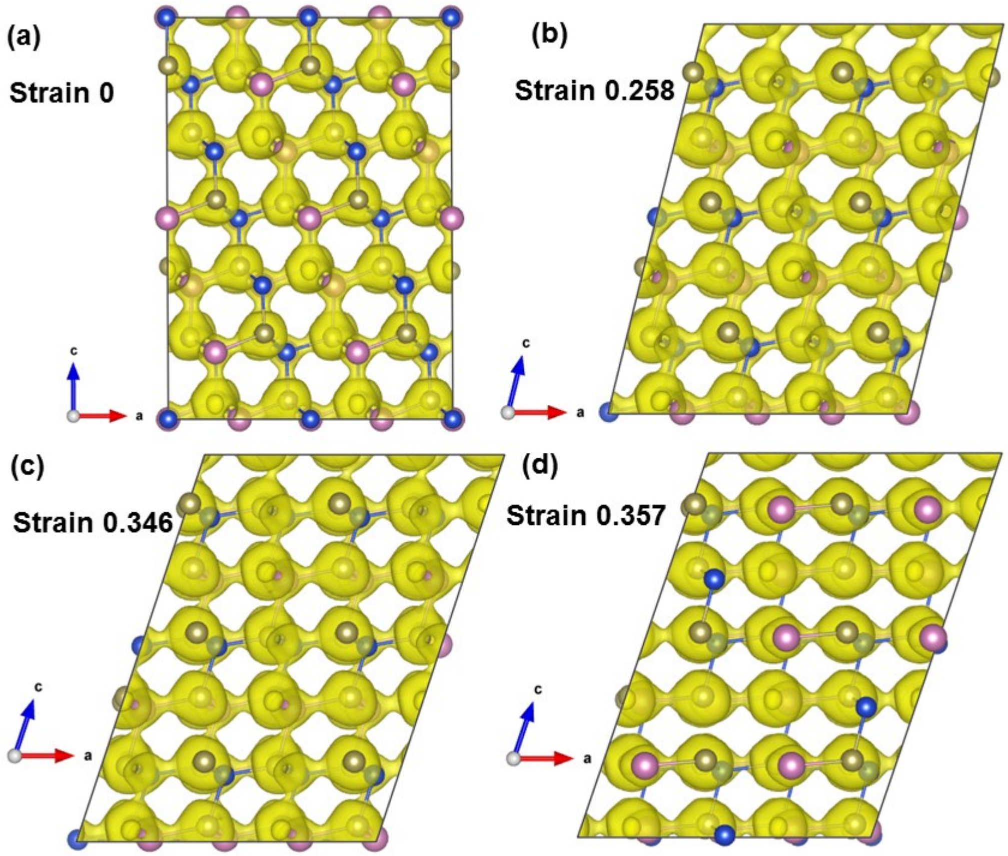

Figure S4. Calculated atomic configurations combined with isosurfaces of the electron localization function (ELF) for biaxial shear loads along the (221)[11-1] slip system: (a) shear strain 0 corresponds to the initial stage, (b) shear strain 0.258 corresponds to the maximum shear stress point, (c) shear strain 0.0.346 before failure, and (d) failure strain of 0.357. The ELF is represented by the shallow yellow region.

REFERENCES:

1. Li, B.; Sun, H.; Chen, C., Large indentation strain-stiffening in nanotwinned cubic boron nitride. *Nat. Commun.* 2014, *5*, 4965.