

Supplementary materials

1. Relaxed configurations of the MgO grain boundary with increasing pressure

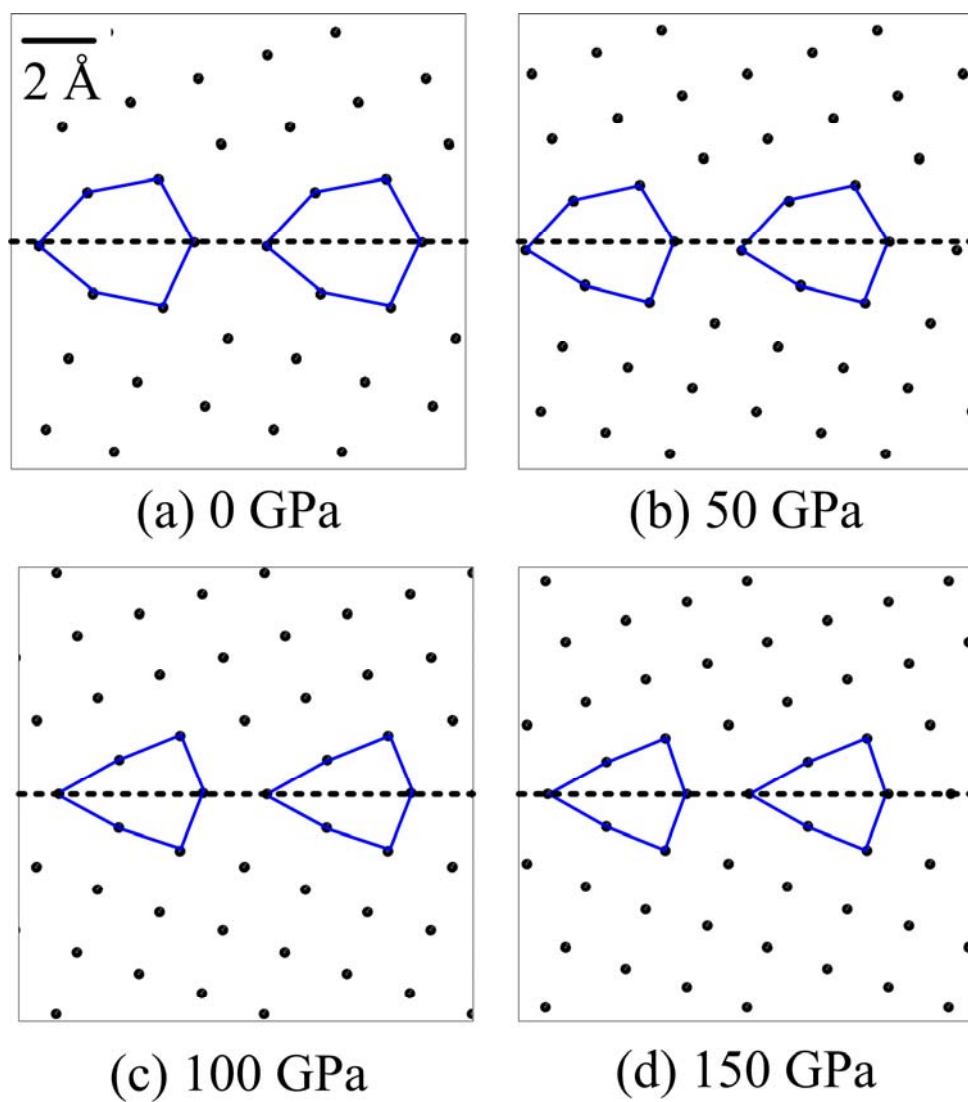


Fig. S1. (Color online) Relaxed configurations of MgO $\{310\}/[001]$ GBs at (a) 0, (b) 50, (c) 100 and (d) 150 GPa pressures. Atoms are represented by black dots, and the atomic structural units composing the boundary are delineated by blue lines.

2. Elastic strain fields at different pressures

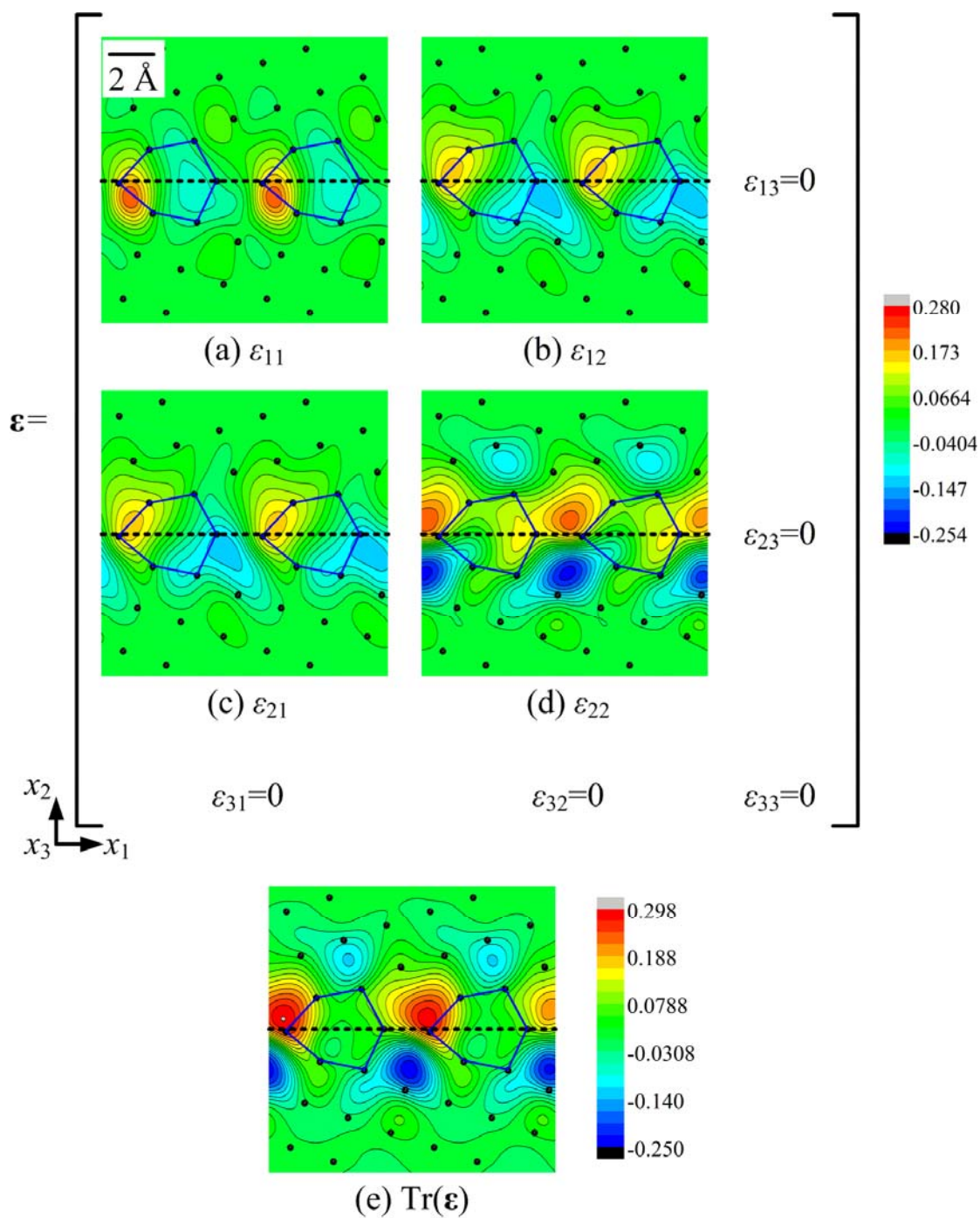


Fig. S2. (Color online) Close-up showing the strain tensor $\boldsymbol{\varepsilon}$ along the boundary at 0 GPa.

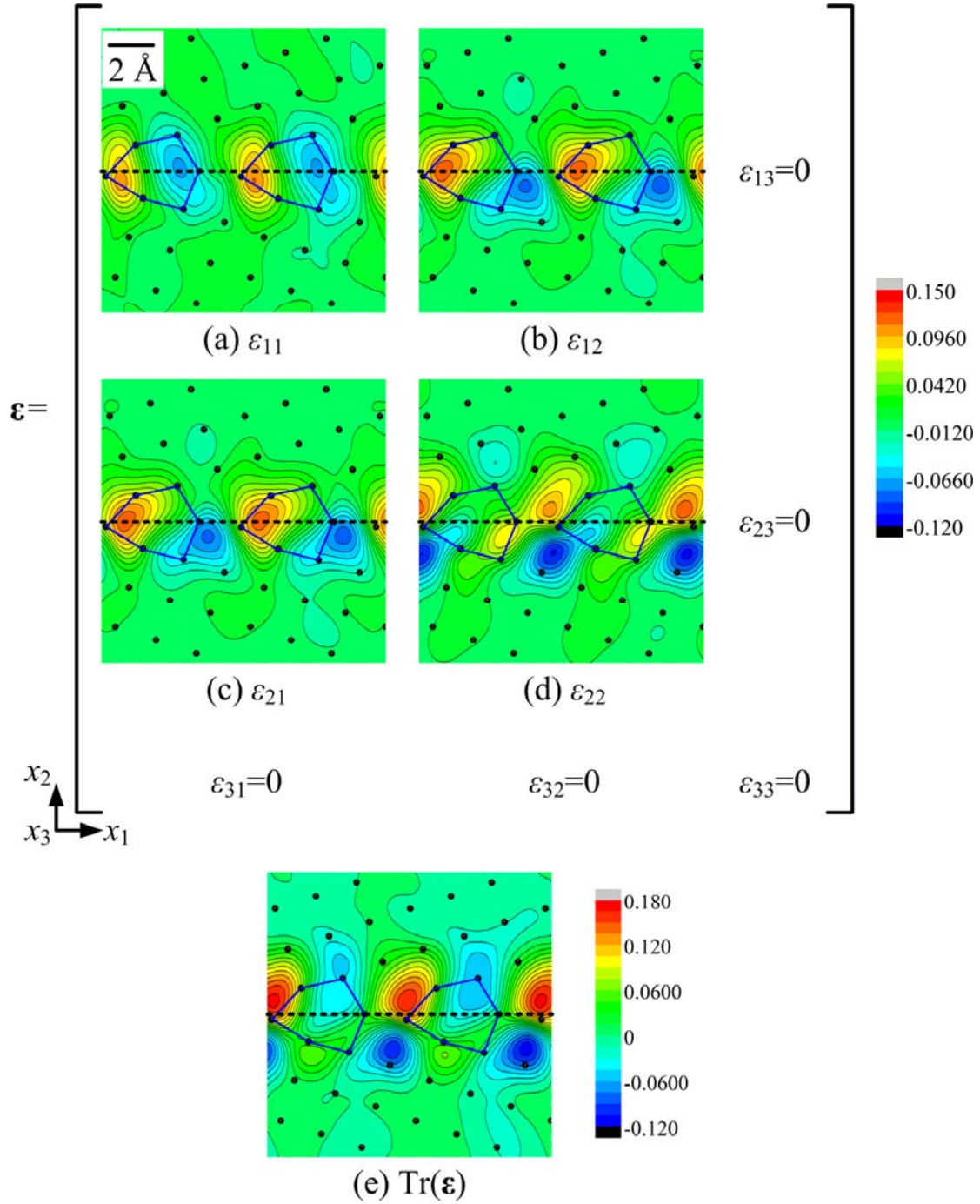


Fig. S3. (Color online) Close-up showing the strain tensor ϵ along the boundary at 50 GPa.

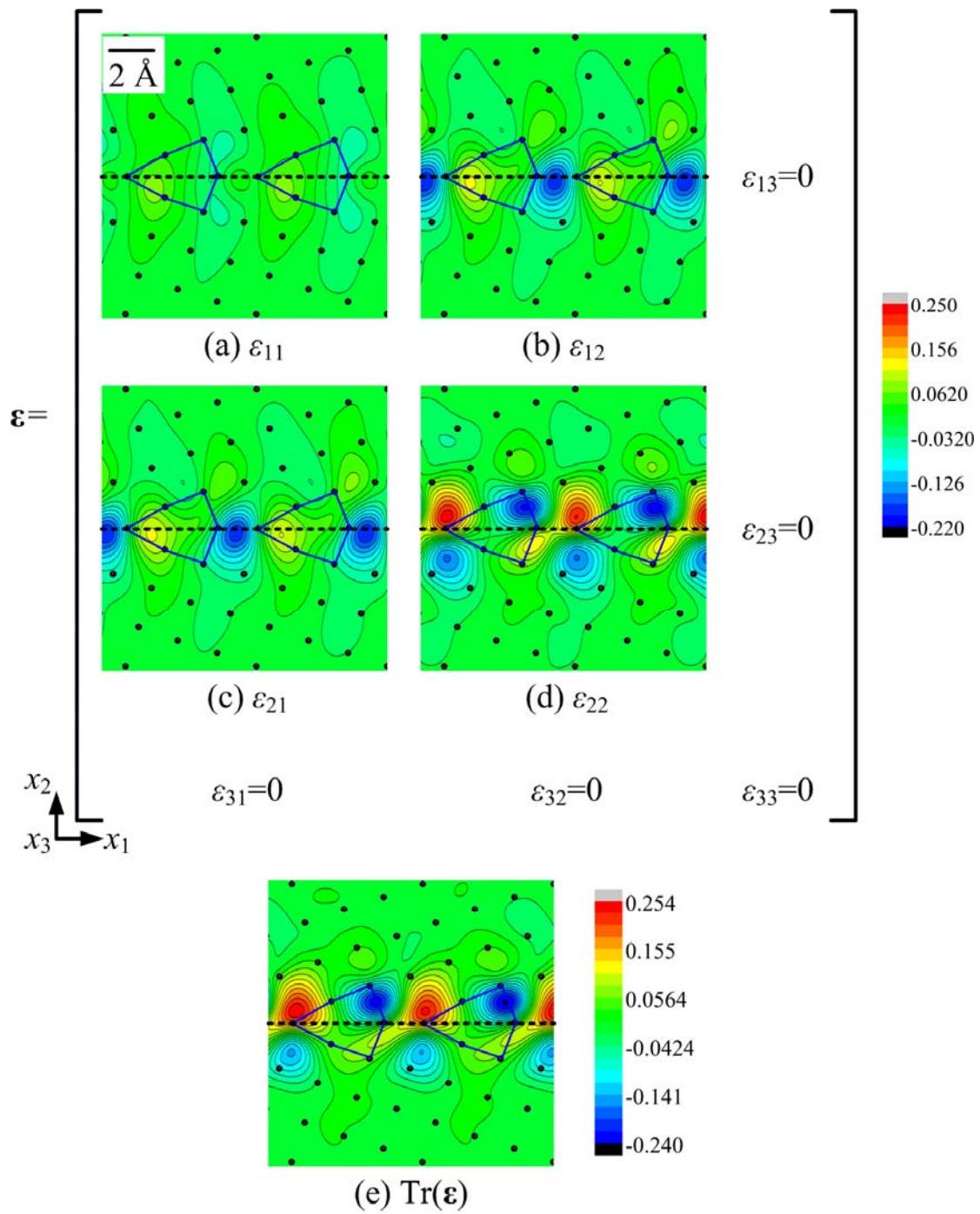


Fig. S4. (Color online) Close-up showing the strain tensor ϵ along the boundary at 100 GPa.

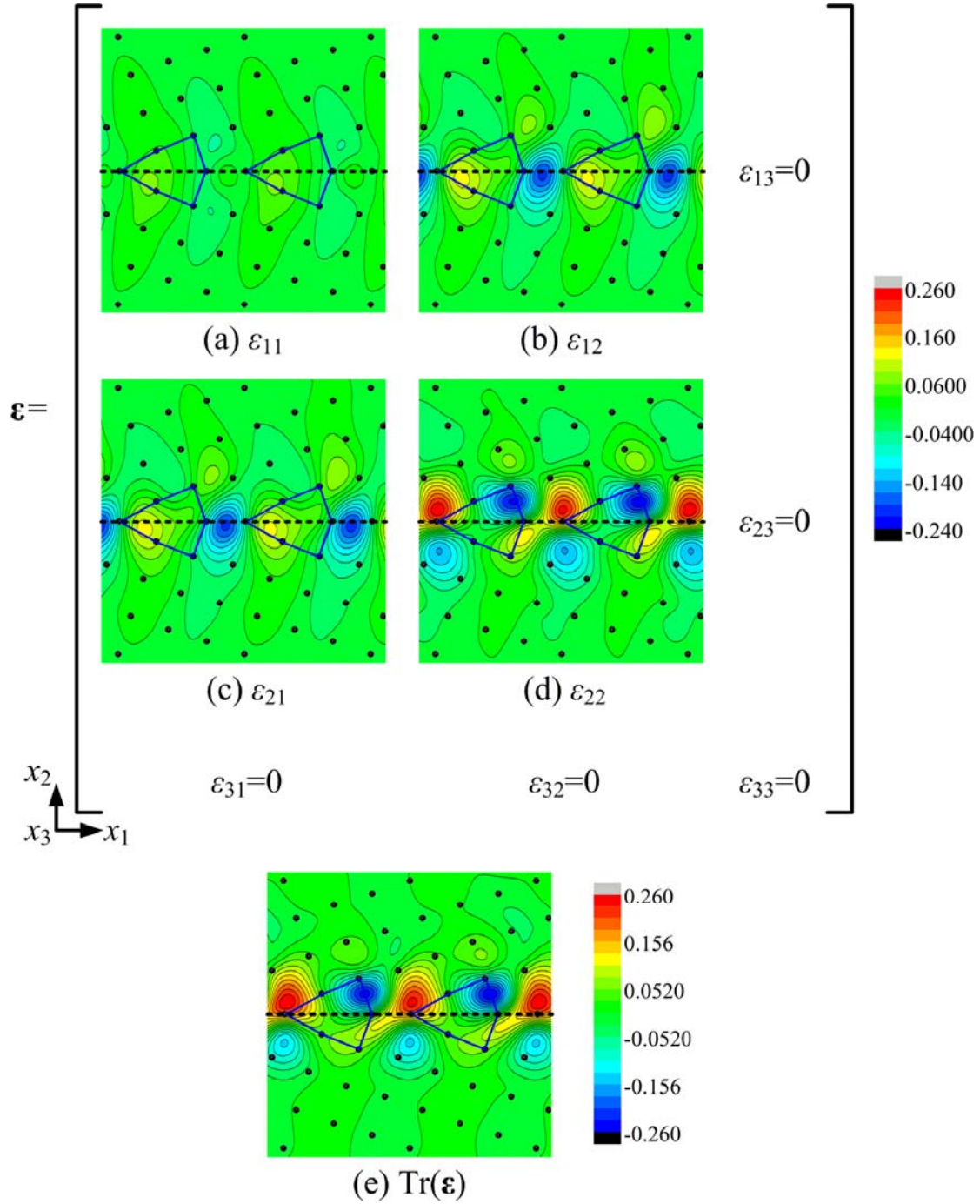


Fig. S5. (Color online) Close-up showing the strain tensor $\boldsymbol{\varepsilon}$ along the boundary at 150 GPa.