Supporting Information

Shear-Induced Brittle Failure along Grain Boundaries in Boron Carbide

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Figure S1

**Figure S1.** The comparison of (a) the angles of C2-B14-C3 and (b) the B166 and B155 bond distances for both GB-I and Fe-doped GB models under pure shear conditions as a function of shear strains.
Figure S2. The GB1 structural evolution of GB-I model under biaxial shear deformation: (a) the intact structure; (b) the structure at 0.136 strain; (c) the structure at 0.155 strain corresponding to the first stress drop; (d) the structure at 0.209 strain corresponding to the maximum shear stress; (e) the failed structure at 0.227 strain. The boron and carbon atoms are represented by the green and sienna balls, respectively.
Figure S3. The GB2 structural evolution of the GB-I model under biaxial shear deformation: (a) the intact structure; (b) the structure at 0.136 strain; (c) the structure at 0.209 strain corresponding to the maximum shear stress; (d) the failed structure at 0.227 strain. The boron and carbon atoms are represented by the green and sienna balls, respectively.
Figure S4. The GB1 structural evolution of the Fe-doped GB model under biaxial shear deformation: (a) the intact structure; (b) the structure at 0.173 strain corresponding to the maximum shear stress; (c) the failed structure at 0.191 strain. The boron and carbon atoms are represented by the green and sienna balls, respectively. The Fe atom is represented by the yellow ball.
Figure S5. The comparison of (a) the B162-B163 bond distance and (b) the C23-B105-C26 chain angle in GB-I and Fe-doped GB models under biaxial shear conditions at various shear strains.
Figure S6. The GB2 structural evolution of Fe-doped GB model under biaxial shear deformation: (a) the intact structure; (b) the structure at 0.173 strain corresponding to the maximum shear stress; (c) the failed structure at 0.191 strain. The boron and carbon atoms are represented by the green and sienna balls, respectively.