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Evolution of Symmetrical Grain Boundaries under External Strain in Iron Investigated by Molecular Dynamics Method

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Abstract: In the present work, the evolution of atomic structures and related changes in energy state, atomic displacement and free volume of symmetrical grain boundaries (GB) under the effects of external strain in body-centered cubic (bcc) iron are investigated by the molecular dynamics (MD) method. The results indicate that without external strain, full MD relaxations at high temperatures are necessary to obtain the lower energy states of GBs, especially for GBs that have lost the symmetrical feature near GB planes following MD relaxations. Under external strain, two mechanisms are explored for the failure of these GBs, including slip system activation, dislocation nucleation and dislocation network formation induced directly by either the external strain field or by phase transformation from the initial bcc to fcc structure under the effects of external strain. Detailed analysis shows that the change in free volume is related to local structure changes in these two mechanisms, and can also lead to increases in local stress concentration. These findings provide a new explanation for the failure of GBs in BCC iron systems.

Keywords: grain boundary; free volume; strain effect; micro-cracking; molecular dynamics

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Table S1. The peak tensile stresses of all cases studied in this work are listed in table.

Model	Strain	Stress/GPa
∑=3(112)	10.65%	13.43
Single crystal	13.50%	16.08
∑=3(111)	13.70%	15.96
Single crystal	22.85%	27.49
∑=5(012)	8.30%	10.098
Single crystal	10.30%	14.3
∑=5(013)	8.50%	9.18
Single crystal	9.25%	11.76
∑=9(221)	9.50%	12.43
Single crystal	16.80%	22.27
∑=11(113)	8.75%	9.27
Single crystal	10.40%	12.89
∑=17(410)	8.15%	9.12
Single crystal	8.90%	10.8

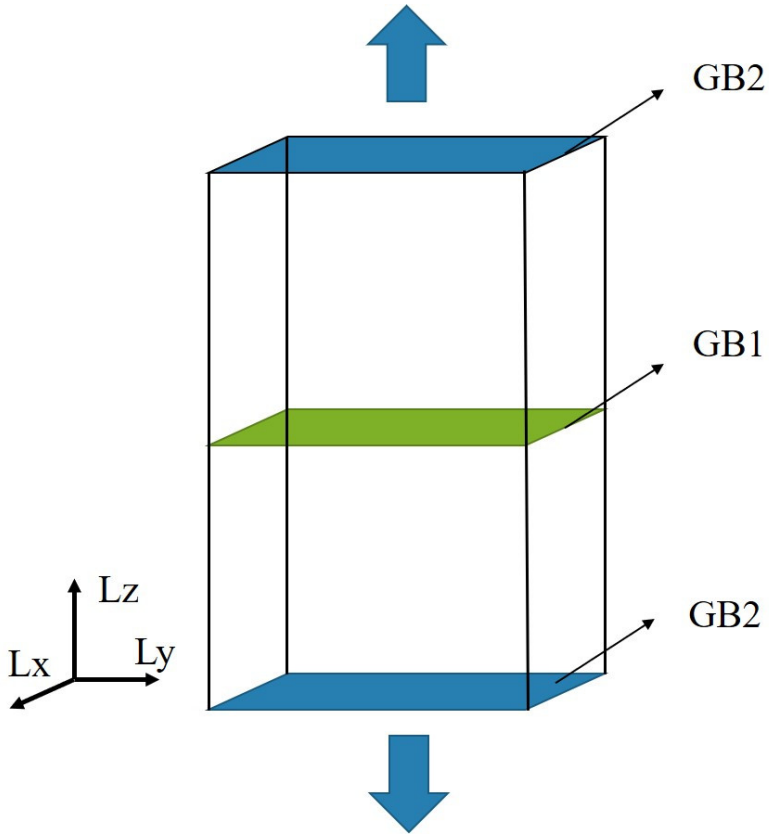

Figure S1. Schematic of grain boundary simulation model used in the present work. For stress-strain simulations, the external tensile strain field is applied on top and bottom surface of box.

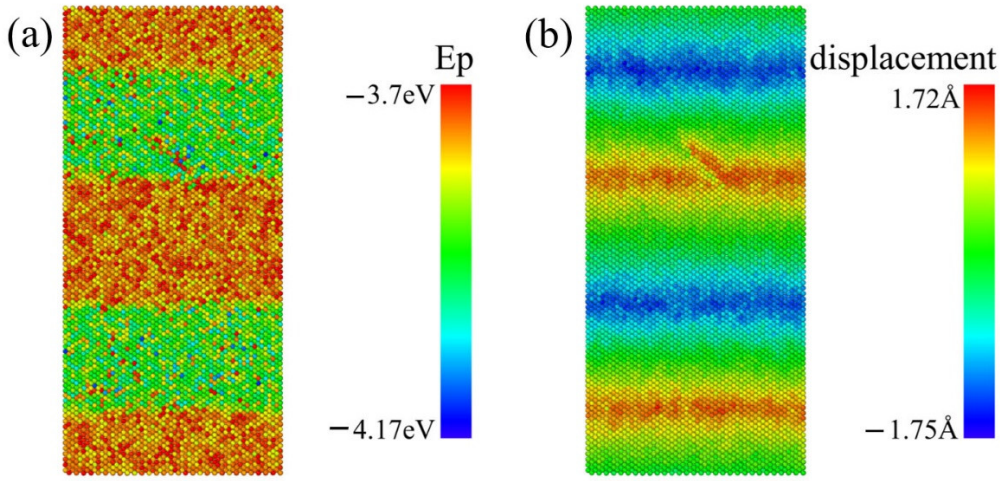

Figure S2. Atomic potential energy (**a**) and displacement distribution (**b**) of ∑3(112) GB at state with peak stress.

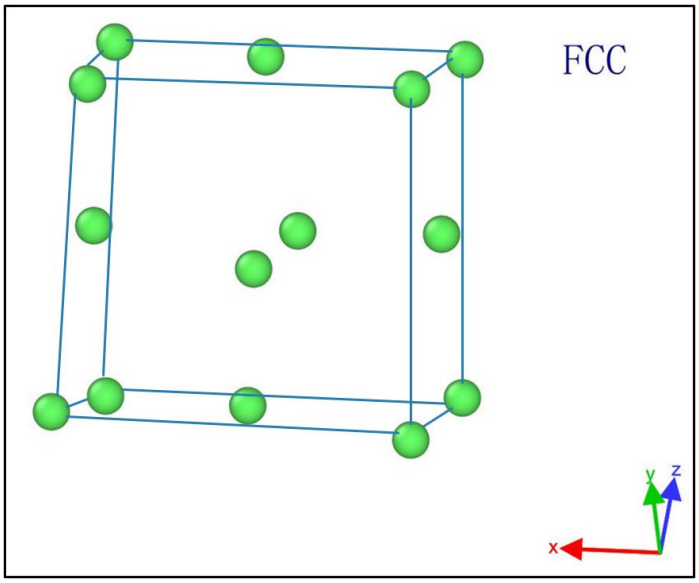

Figure S3. Example of FCC lattice structure in fcc phase after phase transition.

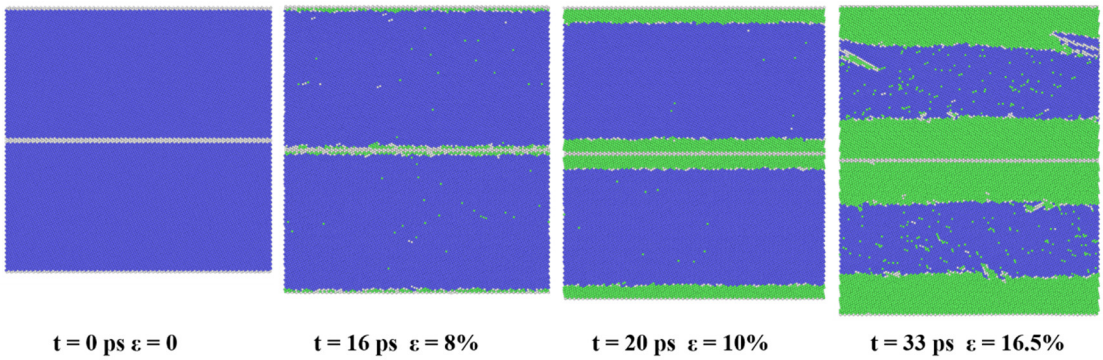

Figure S4. Snapshots (y-z plane) shows ∑ = 5(013) undergoes phase transition and green atom is fcc structure blue atom is bcc. Then the GB happens to crack at 31 ps, region a, b and c are most obvious.

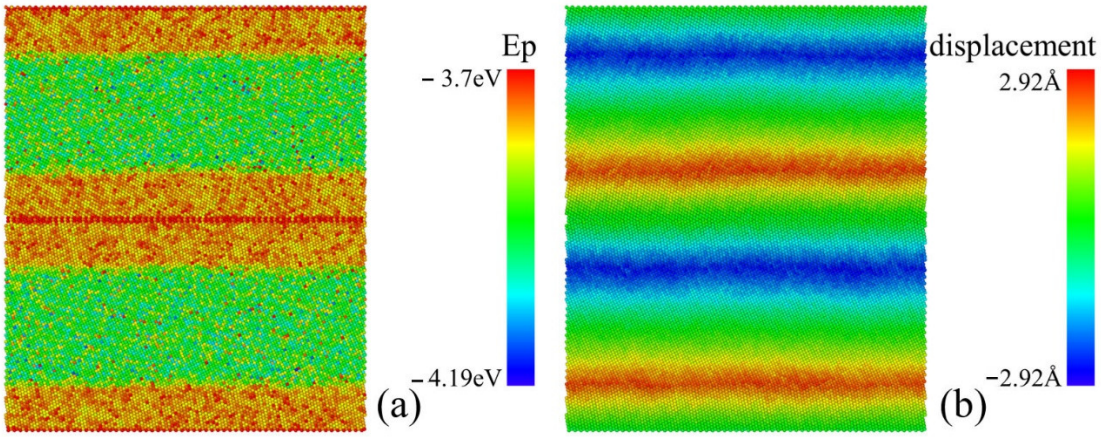

Figure S5. Atomic potential energy (**a**) and displacement distribution (**b**) of ∑5(013) GB at state with peak stress.

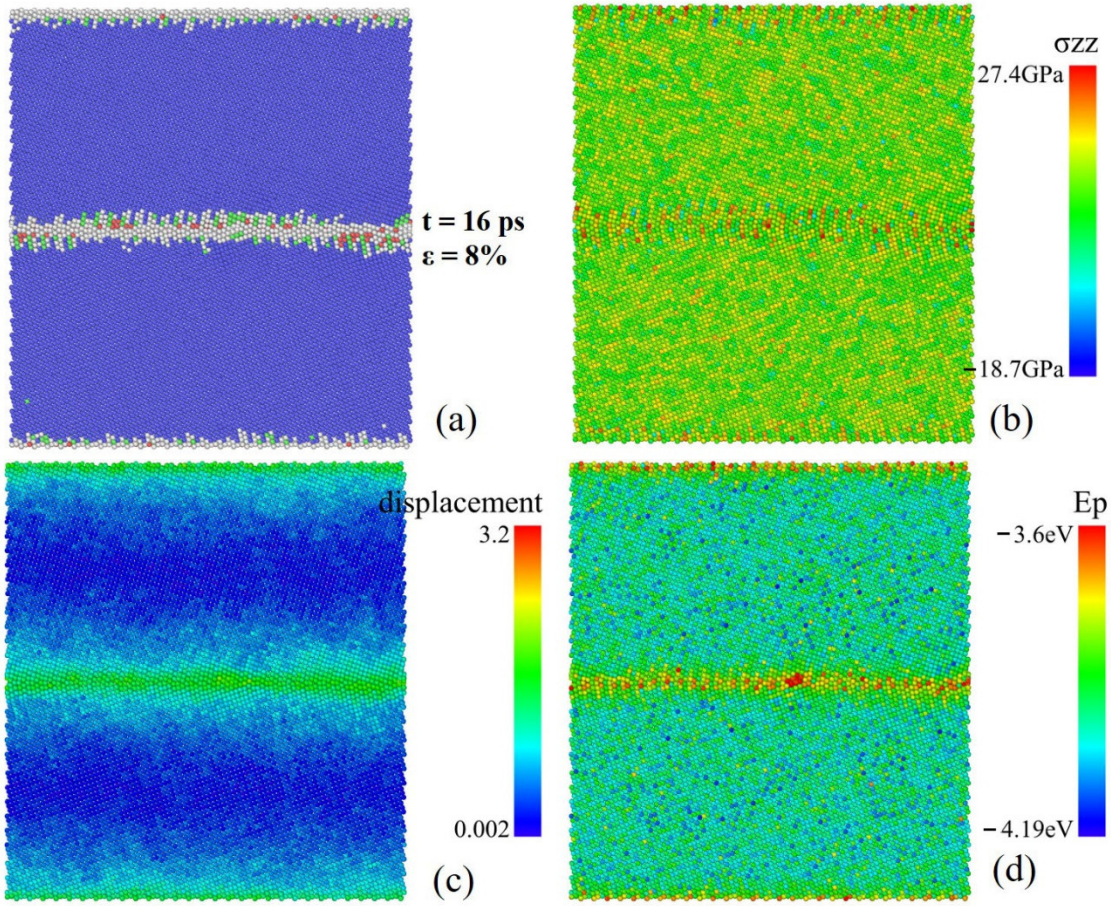

Figure S6. (**a**) The structure of ∑5(012) when slip system is activated with strain around 8%. The potential energy(**b**), stress(**c**) and atomic displacement distribution (**d**) at this state are shown respectively.

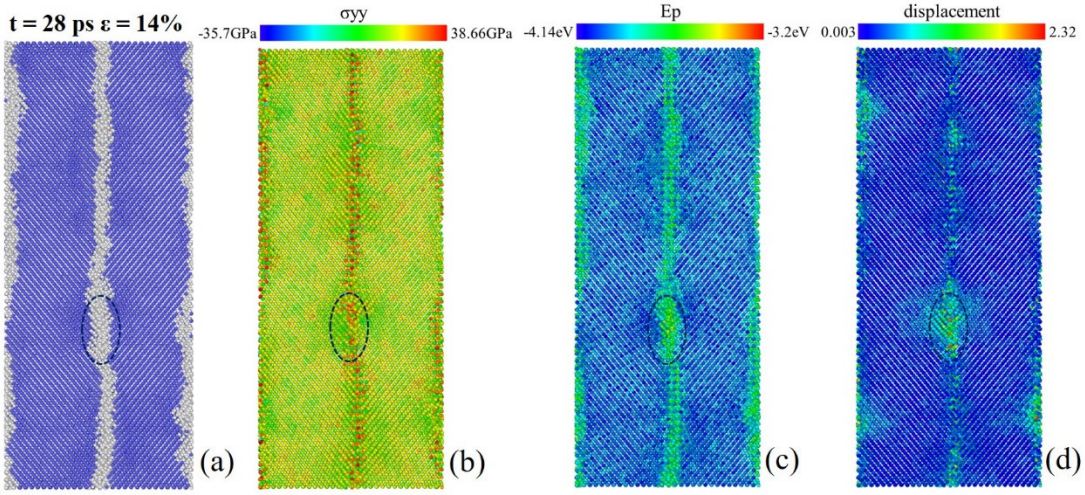

Figure S7. (**a**) The structure of ∑3(111) when slip system is activated with strain around 14%. The potential energy, stress and atomic displacement distribution at this state are shown in (**b**), (**c**) and (**d**) respectively.

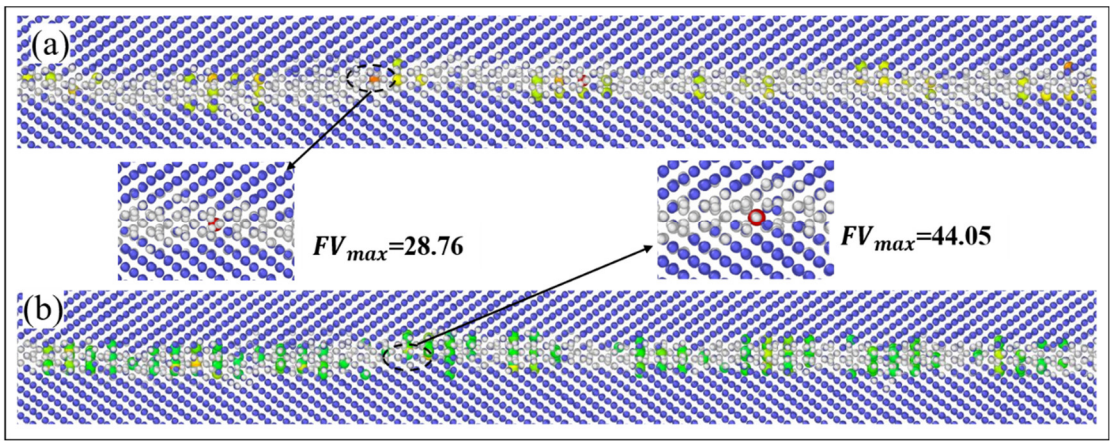

Figure S8. Distribution of free volume near ∑3(111) GB region at (**a**) 0 ps and (**b**) at 28 ps (strain around 14%).