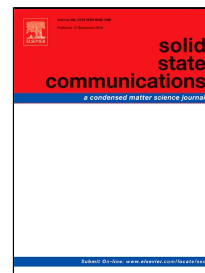


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**Proposed mechanism of twin formation during hexagonal-close-packed structure
to face-centered-cubic phase transition**

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Abstract:

Detailed process, critical energy, and critical shear stress of twin formation during hexagonal-close-packed (HCP) to face-centered-cubic (FCC) transition are proposed through first principles calculation. It reveals that a lower critical energy is needed for HCP→FCC basal transition with twin formation than that without twin. The relative magnitude of critical shear stresses is strongly correlated with c/a ratio of HCP metals, and fundamentally determines the appearance of HCP→FCC basal transition and phase-transition twin. The predicted results bring about reasonable explanations to two puzzling points regarding Mg and twin formation in the literature.

Keywords: A. HCP metals; C. Twin formation; D. HCP→FCC phase transition; E. First principles calculation

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