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Effect of stacking fault energy on the dislocation interaction mechanisms in Cu and Cu-Al alloys: a molecular dynamics study

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We study the effect of stacking fault energy on the deformation behaviour of copper and copper-aluminium alloys using molecular dynamics simulations. We study the interaction of Shockley partial dislocations with twins, stacking faults, and other dislocations. Various interactions occur when the Shockley partial dislocation approaches the twin boundary; secondary twin formation, FCC to HCP transformation, V-shaped twin formation, and repulsion. Furthermore, the interaction of dislocations among themselves leads to complex dislocation networks and affects the formation of deformation twins and de-twinning. We correlate these interaction mechanisms with the stress-strain response of Cu and Cu-Al alloys. Further, to understand the role of stacking fault energy, we compare the interaction mechanisms in Cu and Cu-Al alloys.

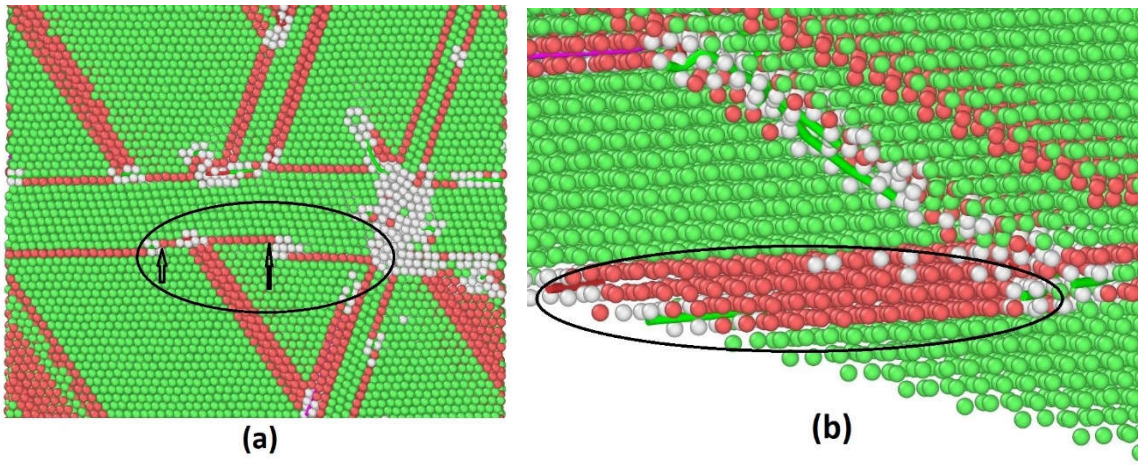

Figure. Interaction of Shockley partials with pre-existing twin leads to (a) step formation at the twin boundary and (b) FCC to HCP transformation. Here green atoms are FCC coordinated, red atoms are HCP coordinated, white atoms are non-coordinated and green lines are Shockley partials.

Keywords: Stacking fault energy; Cu-Al alloy; Molecular dynamics; Loop expansion; Twin boundary; Dislocation interactions.

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