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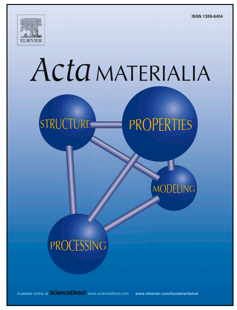

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Unveiling the Role of Super-Jogs and Dislocation Induced Atomic-Shuffling on Controlling Plasticity in Magnesium

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Abstract

Magnesium (Mg) alloys are promising metals for many lightweight structural applications. However, the fundamental deformation mechanism in Mg that lead to poor ductility, formability and anomalous thermal-hardening response remain elusive. Here, atomistic simulations were utilized to unveil the origins of these mechanisms. We show that pyramidal $\langle c + a \rangle$ screw dislocations glide in hexagonal-close packed crystals by a fundamentally new mechanism that involves atomic shuffling and kink pair formation on the trailing partial. Due to local fluctuations in the stresses in the dislocation core, stable super-jogs subsequently form due to inhomogeneities in the shuffling process along the dislocation length as well as due to kink pair collisions. The screw dislocation then moves while dragging these super-jogs, sometimes leaving debris behind (e.g. vacancies or interstitials) as well as long faulted loops on the basal plane that are aligned along the basal plane intersection with the pyramidal-II plane. These dragged out super-jogs dissociate athermally on the basal plane and exert a strong drag-effect on dislocation glide, resulting in dramatic work-hardening at small strains between 0-600K, which correlates with the experimentally observed low-ductility during c-axis compression of Mg. Furthermore, this new mechanism also accounts for the experimentally reported anomalous thermal-hardening as a result of the increase in the number of super-jogs per dislocation unit-length due to thermal activation.

Keywords: Magnesium, Pyramidal Slip, Jogs, Atomic Shuffling, Thermal-Hardening

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