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"Quasicontinuum analysis of dislocation-coherent twin boundary interaction to provide local rules to discrete dislocation dynamics"

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ABSTRACT

The interaction of a pure screw dislocation with a Coherent Twin Boundary Σ3 in copper was studied using the Quasicontinuum method. Coherent Twin Boundary behaves as a strong barrier to dislocation glide and prohibits slip transmission across the boundary. Dislocation pileup modifies the stress field at its intersection with the Grain Boundary (GB). A methodology to estimate the strength of the barrier for a dislocation to slip across CTB is proposed. A screw dislocation approaching the boundary from one side either propagates into the adjacent twin grain by cutting through the twin boundary or is stopped and increases the dislocation pileup amplitude at the GB. Quantitative estimation of the critical stress for transmission was performed using the virial stress computed by Quasicontinuum method. The transmission mechanism and critical stress are in line with the literature. Such information can be used as input for dislocation dynamic simulations for a better modeling of grain boun...

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*SELF-diffusion (Solid state physics)

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Résumé: The interaction of a pure screw dislocation with a Coherent Twin Boundary Σ3 in copper was studied using the Quasicontinuum method. Coherent Twin Boundary behaves as a strong barrier to dislocation glide and prohibits slip transmission across the boundary. Dislocation pileup modifies the stress field at its intersection with the Grain Boundary (GB). A methodology to estimate the strength of the barrier for a dislocation to slip across CTB is proposed. A screw dislocation approaching the boundary from one side either propagates into the adjacent twin grain by cutting through the twin boundary or is stopped and increases the dislocation pileup amplitude at the GB. Quantitative estimation of the critical stress for transmission was performed using the virial stress computed by Quasicontinuum method. The transmission mechanism and critical stress are in line with the literature. Such information can be used as input for dislocation dynamic simulations for a better modeling of grain boundaries. [ABSTRACT FROM AUTHOR]

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