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New theory for crack-tip twinning in fcc metals

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Abstract

Dislocation emission from a crack tip is a necessary mechanism for crack tip blunting and toughening. In fcc metals under Mode I loading, a first partial dislocation is emitted, followed either by a trailing partial dislocation ("ductile" behaviour) or a twinning partial dislocation ("quasi-brittle"). The twinning tendency is usually estimated using the Tadmor and Hai extension of the Rice theory. Extensive molecular statics simulations reveal that the predictions of the critical stress intensity factor for crack tip twinning are always systematically lower (20-35%) than observed. Analyses of the energy change during nucleation reveal that twin partial emission is not accompanied by creation of a surface step while emission of the trailing partial creates a step. The absence of the step during twinning motivates a modified model for twinning nucleation that accounts for the fact that nucleation does not occur directly at the crack tip. Predictions of the modified theory are in excellent agreement with all simulations that show twinning. Emission of the trailing partial dislocation, including the step creation, is predicted using a model recently introduced to accurately predict the first partial emission and shows why twinning is preferred. A second mode of twinning is found wherein the crack first advances by cleavage and then emits the twinning partial at the new crack tip; this mode dominates for emission beyond the first twinning partial. These new theories resolve all the discrepancies between the Tadmor twinning analysis and simulations, and have various implications for fracture behaviour and transitions.

Keywords: Cracks, Dislocations, Fracture, Molecular statics simulations