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# New theory for Mode I crack-tip dislocation emission

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ABSTRACT

A material is intrinsically ductile under Mode I loading when the critical stress intensity $K_{Ie}$ for dislocation emission is lower than the critical stress intensity $K_{Ic}$ for cleavage. $K_{Ie}$ is usually evaluated using the approximate Rice theory, which predicts a dependence on the elastic constants and the unstable stacking fault energy $\gamma_{usf}$ for slip along the plane of dislocation emission. Here, atomistic simulations across a wide range of fcc metals show that $K_{Ie}$ is systematically larger (10–30%) than predicted. However, the critical (crack tip) shear displacement is up to 40% smaller than predicted. The discrepancy arises because Mode I emission is accompanied by the formation of a surface step that is not considered in the Rice theory. A new theory for Mode I emission is presented based on the ideas that (i) the stress resisting step formation at the crack tip creates "lattice trapping" against dislocation emission such that (ii) emission is due to a mechanical instability at the crack tip. The new theory is formulated using a Peierls-type model, naturally includes the energy to form the step, and reduces to the Rice theory (no trapping) when the step energy is small. The new theory predicts a higher $K_{Ie}$ at a smaller critical shear displacement, rationalizing deviations of simulations from the Rice theory. Specific predictions of $K_{Ie}$ for the simulated materials, usually requiring use of the measured critical crack tip shear displacement due to complex material non-linearity, show very good agreement with simulations. An analytic model involving only $\gamma_{usf}$, the surface energy $\gamma_s$, and anisotropic elastic constants is shown to be quite accurate, serves as a replacement for the analytical Rice theory, and is used to understand differences between Rice theory and simulation in recent literature. The new theory highlights the role of surface steps created by dislocation emission in Mode I, which has implications not only for intrinsic ductility but also for crack tip twinning and fracture due to chemical interactions at the crack tip.



## 1. Introduction

The heightened need for reduced energy consumption across many industries drives the search for improvement structural performance and reliability of materials. High structural performance and reliability are achieved with increased fracture toughness. A fundamental requirement for achieving high fracture toughness in crystalline metals is that a material be intrinsically ductile. A crystalline metal is intrinsically ductile if an atomically sharp crack in a loaded material emits dislocation(s) and blunts rather than cleaving and remaining sharp. Specifically, if the Mode I stress intensity factor for emission $K_{Ie}$ is smaller than the Mode I stress intensity factor for cleavage $K_{Ic}$ (Griffith, 1921), then the material will emit dislocations, blunt, and eventually fail by mechanisms that absorb considerable energy. While the overall fracture toughness is

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governed by many larger-scale factors, materials that are intrinsically brittle, i.e. $K_{Ic} < K_{Ie}$, often have insufficient toughness for failure-critical applications. Dislocation emission from the crack tip is thus a necessary precursor to crack tip blunting and toughening, while also representing one of the classical problems in the mechanics of materials.

In light of its practical importance, a number of continuum mechanics models have been introduced to predict crack tip dislocation emission (Argon, 1987; Armstrong, 1966; Kelly et al., 1967; Rice and Thomson, 1974; Schoeck, 1991). The most widely-used model is that by Rice, which is based on a cohesive model for slip displacement ahead of the crack (Rice, 1992). Under Mode II (in-plane shear) loading, Rice showed that emission is controlled by an energy criterion involving the unstable stacking fault (USF) energy $\gamma_{usf}$. The USF is a saddle point on the generalized stacking fault energy surface associated with relative shear displacements of two rigid blocks of material. Under Mode I loading, the Mode II analysis does not apply directly, but Rice postulated that, at the point of emission, the slip profile along the slip plane is the same as that in Mode II. This yields a dependence of $K_{Ie}$ on $\gamma_{usf}$ and on the orientation of the slip plane relative to the crack front.

Molecular statics and dynamics simulations provided a means by which to validate the Rice model. Early simulations (Zhou et al., 1993; Knap and Sieradzki, 1999) showed that the Rice criterion gives accurate predictions for $K_{IIe}$ under Mode II loading, where the crack plane is coplanar with the slip plane. However, results for Mode I loading showed varying levels of agreement from material to material. It was recognized that deviations from the Rice criterion could be due to the creation of a surface step (surface ledge) during the Mode I nucleation process. Several authors thus tried to incorporate the additional energy of the surface step (Gumbsch and Beltz, 1995; Zhou et al., 1994; Xu et al., 1995; Juan et al., 1996) into a Rice-type analysis, but usually for one particular material with some approximations, and without achieving significantly better results. In all of these models, the key Rice concept was maintained: the unstable stacking fault energy controls the dislocation nucleation with emission occurring when the slip displacement reaches the displacement corresponding to the unstable stacking fault displacement. Schoeck (2003) considered a related continuum model, but with creation of a step introduced through an additional constant force acting at the crack tip. The resulting energy functional was then solved approximately using a variational method to obtain the slip distribution along the slip plane, and results were shown for simplified slip energy models. One conclusion of the Schoeck analysis is that, for low step energy, dislocation emission could occur below the Rice prediction, which is not generally supported by simulations in Mode II or Mode I for atomically sharp cracks and is difficult to rationalize physically. Schoeck was pursuing a valuable path that is echoed here, but with an approximate model. Zamora et al. (2012) recently proposed a continuum approach that included extra energy for step formation near the crack tip and proposed a method for computing the step energy contribution, but they presented limited results for a specific system where the role of surface step creation was not clearly identified.

Here, we approach the Mode I emission problem as a mechanical instability governed by a critical crack tip displacement. We show that, in contradiction to a key assumption in the Rice theory, the energy change at the crack tip due to relative slip is monotonically increasing with crack tip displacement, due to the energy cost of creating the step. Thus, the Rice theory simply cannot apply: there is no saddle point in the energy versus slip. We then develop a model that assumes all non-linear response to occur at the crack tip to demonstrate that, in the presence of the step, there exists a critical crack tip displacement at which mechanical instability occurs, i.e. the driving stress at the crack tip due to the applied field can no longer be balanced by the restoring stresses that resist step formation. The simple model rationalizes simulation trends and provides analytic results. We apply the model to 17 different fcc materials where, due to material non-linearities, we use the measured critical crack tip displacement in the theory and then predict $K_{Ie}$ in very good agreement with the simulated values. The new theory captures all key aspects of the Mode I dislocation nucleation process, resolving the discrepancies of the Rice theory. A simplified analytic model is then presented that involves only easily-computable material properties yet shows excellent agreement with the simulations. The simplified model is also used to rectify previous discrepancies between Rice theory and atomistic simulations in other materials.

The remainder of this paper is organized as follows. In Section 2, we give a more detailed exposition of the Rice theory and its predictions for $K_{Ie}$ and the critical slip $\Delta_c$ for elastically anisotropic materials (Sun and Beltz, 1994; Stroh, 1958). In Section 3, we first introduce 17 fcc materials that will be studied, we then carefully validate the Rice model for Mode II loading for these materials, and finally we present results for Mode I loading, with a slip plane inclined at an angle $\theta = 70.53^0$ with respect to the crack plane, and show clear deviations from the Rice theory. In Section 4, we show that the energy change at the crack tip during the emission/slip process has contributions from the surface step energy as well as the stacking fault energy. In Section 5, we developed the new theory for crack tip dislocation emission based on a mechanical instability at the crack tip. In Section 6, we compare the new theoretical model for dislocation emission to simulations across a wide range of fcc materials. In Section 7, we introduce an analytic criteria and show it to be in good agreement with the full model results. Implications of the new model are then discussed and our main results reiterated in Section 8.

## 2. Review of Rice criterion for dislocation emission

Rice formulated a criterion for crack tip dislocation emission based on the Peierls concept (Hirth and Lothe, 1982). This concept assumes the existence of a periodic energy functional $\Psi_{gsf}$ that is a function of the relative slip $\Delta$ between two rigid crystal blocks. The energy $\Psi_{gsf}$ is the so-called generalized stacking fault energy (GSF energy) evaluated at relative slip $\Delta$, with $0 \leq \Delta \leq b$ where $b$ is the Burgers vector of the emitted dislocation. For fcc materials, the focus of the work here, the emitted dislocation is a partial dislocation with Burgers vector $b_p$. The emission of the partial dislocation leaves behind a stable stacking fault as the dislocation glides away from the crack tip. A typical GSF energy function is shown in Fig. 1,