Crack Tip Enhanced Crystal Plasticity Phase Field Model for Crack Propagation in Ti64 Alloys

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Abstract
This work introduces a computational fracture model for Ti64 alloy that is based on coupled Crystal Plasticity Phase Field model for fracture but also considers the atomistic mechanisms of plasticity at the crack tip. Atomistic simulations are conducted to identify the crack-tip mechanisms of plasticity and the continuum scale phase field model is augmented to account for this.

1. Introduction

Phase field models have been used to predict crack growth and propagation in metals with good accuracy. Consider a polycrystalline specimen in some loading conditions. Within a grain, the material deforms by elastic stretching as well as plastic deformation due to dislocation motion. At this stage dislocation density mainly evolves through dislocation loop expansion and interaction. The interaction of these dislocations creates regions of potential microcracks. The dislocations around the microcrack are either annihilated at the free surface or driven away due to the high stresses in the crack region, creating a temporary dislocation-free zone. Upon further loading, the crack itself becomes a source of dislocations as new dislocations nucleate from the tip. Continuum scale fracture models do not account for these dislocations are they are only captured in atomic-scale simulations. Atomistic simulations on the other hand are limited by time and length scales. This work describes the use of Atomistic scale simulations to study crack-tip plasticity and enhance the coupled Crystal Plasticity Phase Field model, to account for these crack-tip nucleated dislocations.

2. Methodology

The enhancement of defect energy in the Phase Field model is achieved through a five-step process:

i) **Data generation**: Atomistic simulations of a specimen with different crack orientations under varying strain rate conditions are conducted. The evolution of dislocation density with various state variables including principal stresses, effective plastic strain, and strain rate are recorded. For this, the concurrent Atomistic Crystal Plasticity model described in [1] is used, which can transfer discrete dislocations in the MD region to dislocation densities in the continuum region enabling us to study the evolution of dislocation densities from crack-tip.

ii) **Finding critical phase field value s_c**: To indicate the critical stress state at which dislocations start nucleating from the crack tip, the phase field value, which represents cracked regions, is used here. To find s_c, a simulation is conducted on a thin rectangular specimen with a center crack using both the coupled Crystal Plasticity Phase Field (CPFE-PF) model for fracture and the concurrent Atomistic Crystal Plasticity (CPFE-MD) model. The equivalent virial stress at which dislocations nucleate is noted. The phase field value at which the crack-tip equivalent stress in the CPFE-PF simulation reaches this equivalent virial stress is considered s_c.

iii) **Finding critical state variables**: In this step, the most important state variables which affect the dislocation density need to be identified. For this, Bayesian Inference is employed here. The range of dislocation density data obtained is divided into 10 classes or regions which converts the problem into a classification problem. A uniform prior is used for each class of dislocation density. Accuracy is measured using the objective function, which is the probability that a state variable classifies accurately. It was found that dislocation density is most affected by the effective plastic strain and strain rate.

iv) **Finding the form of dislocation density**: The next step is to find the functional form of dislocation density evolution in terms of the dependent state variables found in step (iii). For this, Genetic Programming based Symbolic Regression (GPSR) is used. Data obtained in step (i) is fed into

Eureqa, a software for conducting GPSR analysis, to obtain the equation for dislocation density evolution.

v) **Modifying the CPFE-PF model**: The CPFE-PF model is enhanced with this additional plasticity. This enhancement is done only at the crack tips which are identified using the phase field and its gradient. In the crack-tip, the accumulated slip is augmented by slip due to nucleated dislocations which is given by Orowan's equation.

$$\gamma_{total}^{\alpha} = \gamma_{ssd}^{\alpha} + \rho^{\alpha} b^{\alpha} v^{\alpha}$$

where,

γ_{ssd} = Slip due to pre-existing dislocations, ρ = Dislocation density at crack-tip, b = Burgers Vector, v^{α}=Velocity of dislocation for slip system 'α' (Calibrated using MD)

3. Results

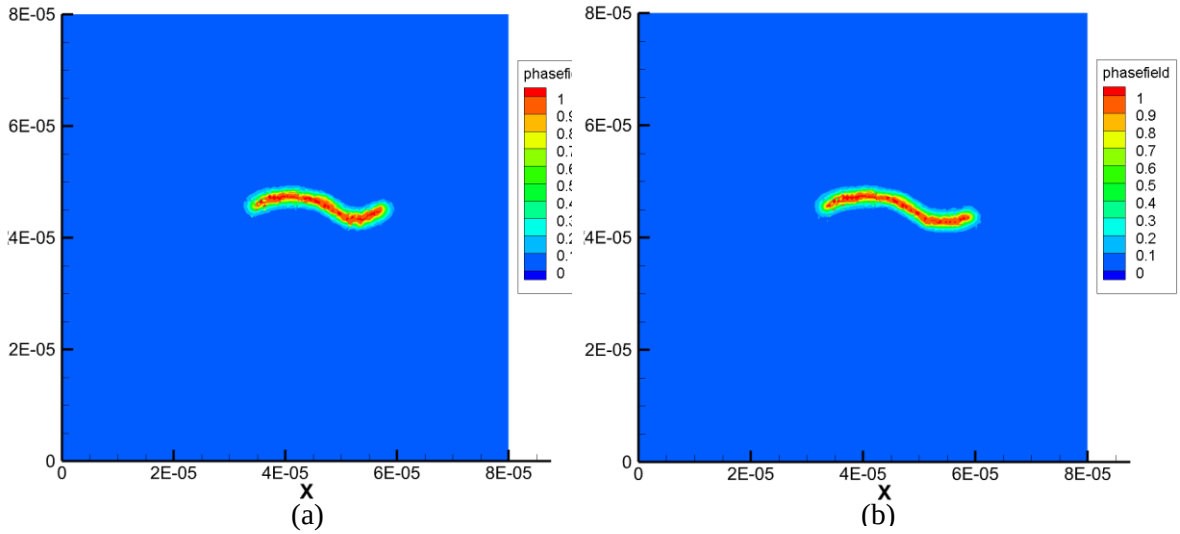

Fig.1 – Difference in the crack path (a): without additional dislocations, (b): with additional dislocations

The evolution of the phase field which represents the crack path and rate of crack propagation is compared with and without the contribution of additional dislocations. The comparison was made using a 41-grain polycrystalline sample with a through-thickness crack at a grain boundary. The comparisons show that the crack path and rate of crack propagation show deviation from the simulation conducted using the model without crack-tip enhancement. The evolution of effective plastic strain at the crack-tip is also higher for the crack tip enhanced model. The additional effective plastic strain at the crack-tip due to nucleated dislocations are compared between the enhanced CPFE-PF model and CPFE-MD model for validation. The evolution of additional effective plastic strain shows good agreement between the models.

4. Conclusions

A crack-tip enhanced coupled Crystal Plasticity Phase Field model for crack propagation is introduced through this work. Comparison with the model without crack-tip enhancement shows a difference in the crack path as well as the rate of crack propagation. The additional plasticity at the crack tip is calibrated and validated using atomic-scale molecular dynamic simulations.

References

[1] Chakraborty, S., Ghosh, S. (2021). A concurrent atomistic-crystal plasticity multiscale model for crack propagation in crystalline metallic materials. *Computer Methods in Applied Mechanics and Engineering*, *379*, 113748.