MICROSTRUCTURECRACK PATH PREDICTION USING GRAPH THEORY

Veera Sundararaghavan, University of Michigan Ann Arbor
veeras@umich.edu

Key Words: high cycle fatigue, in-situ loading, cohesive energy, grain boundary energy, Griffith theory.

The crack path in crystalline metals is determined by the relative strength and orientation of their multiple cleavage directions with respect to the loading direction. The strength of the cleavage surfaces depend on the local chemical environment and crystallographic orientation of the interfaces. Understanding the cohesive energy in a polycrystalline metal is fundamental to predicting its susceptibility to failure mechanisms such as cracking and fatigue. In a recent work, we studied a geometric method based on Wulff's diagram of inverse cohesive energy to predict fracture [1]. We find the existence of forbidden regions where cracks cannot propagate, and often the presence of multiple optimal crack propagation angles in which case the crack path's local orientation switches rapidly to follow the microscopically preferred path. This behavior results in saw-tooth patterns on the fatigue cracks. We introduce a novel approach based on multiscale graph theory to predict such paths of microscale cracks in polycrystalline materials. We represent the crack path as the boundary of a partition in a geometric graph, obtained by optimizing an Ising-type hamiltonian. The hamiltonian parameters are chosen so that the partition cost equals the energy of the corresponding crack. The growth angle of the crack in polycrystalline materials is influenced by the loading conditions and the microstructure near the crack tip. To account for this, we incorporate two length scales, macro and micro, and define the total energy of the crack as the sum of macroscopic energy release and microscopic surface energy. The former guides the crack to propagate along the direction of maximum energy release, while the latter directs the crack along the macroscopically preferred direction. The crack path accommodates both intergranular and transgranular fractures, with the former occurring along grain boundaries and the latter along crystallographic cleavage planes. We study mixed-mode fracture in a thin foil specimen and include the dihedral angle of the 2D crack to define effective surface energy. We validate our model using analytical results for mixed-mode fracture in an isotropic medium and mode-I fracture in a medium with a preferred crack direction. Finally, we compare our results against thin foil experiments on a HCP Magnesium alloy. Overall, our approach can aid in designing materials with optimal fracture resistance by controlling their microstructure.

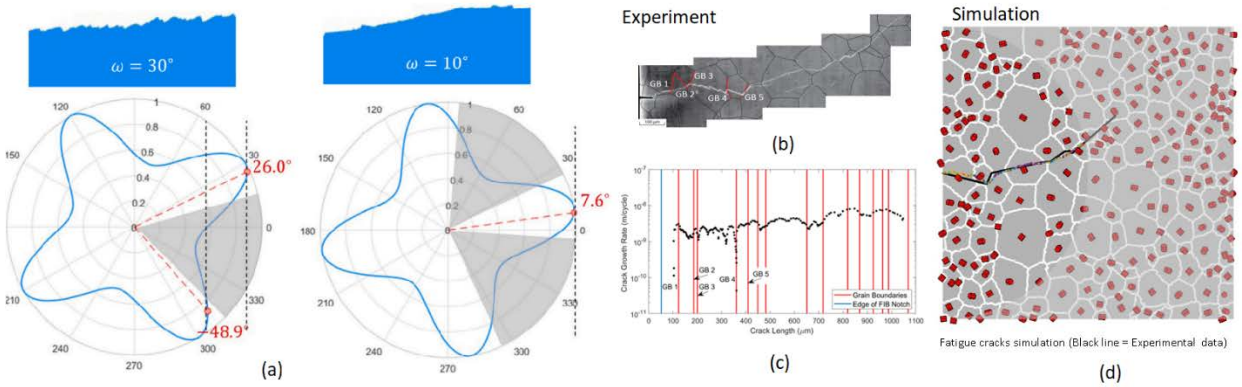

Figure.1 (a) Wulff plots show the inverse of surface energy of two planar crystals of differing orientation (30 and 10 degrees). The gray areas indicate forbidden regions of fracture. In the first case, the crack is predicted to follow a zig zag path at two angles. (b) Experimentally observed crack path in a foil specimen. (c) measured growth rate of the crack indicating pauses at the grain boundary (d) Crack path predicted by the graph model matches experimental data

Reference [1] Srivastava, S., Yaghoobi, M. and Sundararaghavan, V., 2021. A graph-theoretic approach for multiscale modeling and prediction of crack propagation in polycrystalline materials. Engineering Fracture Mechanics, 241, p.107406.