Finite Element-Based Model for Crack Propagation in Polycrystalline Materials

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ABSTRACT

A two-dimensional numerical model for crack propagation through polycrystalline microstructures is proposed. The extended finite element method (X-FEM) [1] is adopted as the computational method of choice. The X-FEM is a recently proposed numerical method which facilitates crack propagation simulations to be conducted without explicitly meshing the crack surfaces or the need to remesh as the crack advances. In the X-FEM, the finite element space is enriched by adding special functions to the approximation through the notion of partition of unity. For crack problems, the Heaviside step function and the elastic asymptotic near-tip displacement fields are used as enrichment functions. A Galerkin procedure is adopted to obtain the discrete equations.

Polycrystalline materials are comprised of grains whose boundaries play a key role in the thermodynamic and mechanical processes operating at the microscale, and hence it is evident that the properties of grain boundaries and interfaces play a significant role in the failure mechanisms in these classes of materials. In this study, we incorporate grain boundary characteristics within a finite element-based model to explore dominant fracture modes in polycrystalline materials. Polycrystalline microstructures are generated using the Potts model for grain growth. The microstructural calculations are carried out on a regular lattice and a constrained Delaunay triangulation algorithm is used to construct the initial finite element mesh of the microstructure [2]. The fracture properties of the microstructure are characterized by assuming that the critical fracture energy of the grain boundary ($\mathcal{G}_c^{gb}$) is different from that of the grain interior ($\mathcal{G}_c^i$). The crack is assumed to propagate along a grain boundary or through the grain interior depending on which has the larger value of $\mathcal{G}/\mathcal{G}_c^k$ (k is either gb or i). Numerical crack propagation simulations for varying toughness ratios G_c^{gb}/G_c^i are presented, to study the competition between intergranular and transgranular modes of crack growth. The ease and capability of modeling brittle fracture through a microstructure is realized, which opens-up the possibility to integrate experiment-and-computation in engineering microstructures for improved toughness.

References

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