20th European Mechanics of Materials Conference - EMMC20
Florence, Italy | May 27th-29th, 2026
www.emmc20.unifi.it

From lattice structure to fracture toughness in brittle solids

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Paper ID: 439
Symposium S8: Fracture, and damage of materials
Extended Abstract

Abstract

Fracture toughness and fracture energy are two key, interrelated parameters that characterize a material's resistance to failure. Predicting its value from the solid structure at the atomistic scale remains elusive, even in the simplest situations of brittle fracture. Here we examine the atomistic scale dependence of a material's resistance to failure by numerical simulations and analytical analysis in electrical analogs of brittle crystals. Fracture energy is determined from Griffith's analysis of energy balance during crack propagation, and fracture toughness is determined from fits of the displacement fields with Williams' asymptotic solutions. Significant size dependencies are evidenced in small lattices, with fracture energy and fracture toughness both converging algebraically with system size toward well-defined material-constant values in the limit of infinite system size. The convergence speed depends on the loading conditions and is faster when the symmetry of the considered lattice increases. The material constants at infinity obey Irwin's relation and properly define the material resistance to failure. However, they are incompatible with Griffith's relationship. We show that this deviation is a consequence of the lattice discreetness and decreases when the super-singular terms of Williams' solutions (absent in a continuum medium but present here due to lattice discreetness) are taken into account. The generic asymptotic form taken by this field near the crack tip provides a solution for this matching, and subsequently a way to predict toughness from the atomistic parameters with application to graphene.

Keywords:

Fracture toughnesse Facture energy Williams expansion Fuse model Lattice discreetness