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Fracture of solar-grade anisotropic polycrystalline Silicon: A combined phase field–cohesive zone model approach

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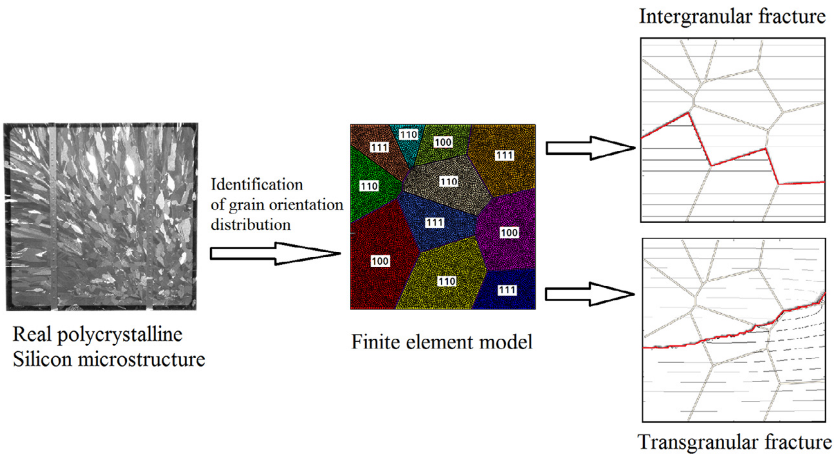
Graphical Abstract



Highlights

- Combined phase-field and cohesive zone model for fracture.
- Transgranular and intergranular fracture in solar-grade Silicon.
- Anisotropic phase field model for fracture.
- Identification of polycrystalline Silicon mechanical parameters.

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Abstract

This work presents a novel computational framework to simulate fracture events in brittle anisotropic polycrystalline materials at the microscopical level, with application to solar-grade polycrystalline Silicon. Quasi-static failure is modeled by combining the phase field approach of brittle fracture (for transgranular fracture) with the cohesive zone model for the grain boundaries (for intergranular fracture) through the generalization of the recent FE-based technique published in [M. Paggi, J. Reinoso, Comput. Methods Appl. Mech. Engrg., 31 (2017) 145–172] to deal with anisotropic polycrystalline microstructures. The proposed model, which accounts for any anisotropic constitutive tensor for the grains depending on their preferential orientation, as well as an orientation-dependent fracture toughness, allows to simulate intergranular and transgranular crack growths in an efficient manner, with or without initial defects. One of the advantages of the current variational method is the fact that complex crack patterns in such materials are triggered without any user-intervention, being possible to account for the competition between both dissipative phenomena. In addition, further aspects with regard to the model parameters identification are discussed in reference to solar cells images obtained from transmitted light source. A series of representative numerical simulations is carried out to highlight the interplay between the different types of fracture occurring in solar-grade polycrystalline Silicon, and to assess the role of anisotropy on the crack path and on the apparent tensile strength of the material.

Keywords: Cohesive zone model; Phase field modeling of fracture; Anisotropic elasticity; Solar-grade polycrystalline silicon; Finite element method

1. Introduction

Accurate prediction of failure in solids is a matter of a great relevance in different industrial sectors ranging from aerospace and aeronautics to renewable energy. At the macroscopic scale, fracture is generally originated by several microscopic defects, i.e. voids and cracks, which grow and coalesce leading to the deterioration of the overall material properties and the load carrying capacity of the structural component. In particular, at the microscopic scale, the interplay between intergranular (cracks propagating along grain boundaries) and transgranular (cracks propagating through the grains) fracture in polycrystalline materials is of major concern in material science and engineering applications.

In the related literature, simplified models specific for intergranular fracture have been proposed in [1–5] based on the cohesive zone model (CZM) inserted along the internal grain boundaries. Cohesive crack formulations can be understood as phenomenological models in which fracture events are triggered by evaluating a particular traction–displacement law. This numerical technique inherently incorporates a characteristic length scale and has been widely used to simulate damage in polycrystalline materials [6], though crack paths are constrained along element edges, see a wide discussion in [7–9], among others.

However, transgranular fracture is also a relevant failure mode in some materials and, in many cases, it is developed in competition with intergranular failure. Therefore, the development of numerical techniques that allow a reliable modeling of grains cracking with arbitrary failure paths are indeed necessary to provide a comprehensive simulation tool. In practical situations, for instance in micro-electro-mechanical systems (MEMS), both types of crack propagation have been reported in [10,11]. In those investigations, the authors comprehensively document the importance of considering the in plane grain anisotropy of Silicon which notably affects the fracture behavior. More specifically, regarding photovoltaics systems, solar-grade polycrystalline Silicon with grains randomly oriented in 3D are frequently used to manufacture thin solar cells. In such a case, both intergranular and transgranular fracture have been experimentally reported [12,13], see also some crack patterns in Fig. 1 experimentally observed by the present authors in solar cells embedded in photovoltaic modules, using the electroluminescence technique. A first attempt to model both types of fracture has been pursued in [14] by an intrinsic cohesive zone model approach. To avoid mesh dependency and un-physical material compliances, the extrinsic approach could be put forward, as in [15]. However, for very brittle materials like Silicon, cohesive zone model approaches suffer from the complexity in resolving the process zone which is very small as compared to the grain size or to the specimen size.

In contrast to the previous numerical methods relying on cohesive zone models only, several studies have also been proposed to account for transgranular crack propagation in polycrystals by means of the extended finite element