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Computational multi-scale and multi-physics methods for the prediction of fracture processes in photovoltaic systems

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Abstract. Renewable energy plays a key role in socio-economic development, driven by the need to reduce energy deficits, with photovoltaic (PV) technology being the dominant option. This study proposes a numerical approach based on the finite element method to assess the impact of cracks in solar cells on the mechanical response of photovoltaic panels. Specifically, polycrystalline Silicon (SiSC) laminates are analyzed. The proposed computational scheme integrates the solid-shell element formulation with the Phase-Field (PF) technique for fracture modeling. The process begins with a large-scale global finite element model of the composite laminate for structural analysis. Subsequently, the displacements calculated at the edges of each solar cell are transferred, through a projection scheme, as boundary conditions to a small-scale 3D local finite element model of the laminates. In this direction, a series of representative numerical simulations are conducted to evaluate the durability of PV modules under bending conditions, providing a robust framework for improving the design and sustainability of these systems.

Keywords: Finite element method; Nonlinear continuum mechanics; Photovoltaic panel laminate; Global/local modeling

1 Introduction

The urgent demand for the development of clean energy sources has motivated extensive research efforts across various fields. In this context, photovoltaic (PV) technology for electricity production can be considered a key technology for developing a decarbonized energy sector [1]. Solar cells based on Silicon (SiSC), are currently a mature technology widely exploited in different applications. Crystalline Silicon PV technology, including monocrystalline and polycrystalline Silicon, represents over 90% of the total production [2].

In the context of fracture events, particularly in polycrystalline Silicon solar cells, the propagation of microcracks represents a major limitation on the electrical efficiency of PV modules during their operational lifespan. On the one hand, the production process of SiSC inherently introduces permanent deformations and residual stresses in the cells before lamination, arising from various stages such as co-firing, flattening, and soldering. On the other hand, during service, PV modules are subjected to various loading scenarios that can initiate microcracks. These microcracks can lead to substantial power losses by isolating damaged areas of the solar panel, sometimes requiring component replacement [4].

At the SiSC level, fracture behavior is characterized by two main failure mechanisms: (i) intergranular cracks along grain boundaries between adjacent crystals and (ii) transgranular cracks that fracture the grains. For micromechanical numerical analysis, (mostly using the finite element method, FEM), polycrystalline SiSCs are typically modeled either by direct image processing [5] or by implementing statistical distributions through Voronoi tessellations.

In order to account for fracture phenomena, the cohesive zone model (CZM) has become a widely used computational approach especially for triggering intergranular cracking phenomena [6]. CZMs have also been extensively applied to simulate transgranular microcracking in polycrystalline materials. In this concern, Mariani et al. [7, 8] developed a multiscale-CZM approach to numerically capture the transgranular failure events in polycrystalline Silicon microelectromechanical systems (MEMS). However, directly applying CZMs to model both failure mechanisms in PV modules presents significant challenges, such as the complex polycrystalline structure of SiSC, the anisotropic nature of Silicon, and the scale of a complete PV module comprising multiple solar cells. In contrast, methods such as the extended element method (XFEM) and the generalized finite element method [9] also enable crack modeling, though accurately identifying crack initiation and paths remains challenging. To address the limitations of these explicit modeling methods for complex crack topologies, the phase field (PF) approach, based on Griffith's theory, has been proposed for modeling cracks in quasi-brittle materials such as Silicon solar cells [10].

In recent years, efforts to reduce production costs of Silicon solar panels have led to a decrease in cell thickness from 300 μm to 150 μm [11], resulting in higher breakage rates and increased crack events. Building on the computational framework in [12], the solid shell formulation combined with an anisotropic phase field model at finite deformation has been proposed to model preferential crack propagation in thin-film solar cells [13, 14].

The complex behavior of PV systems, involving multiple observation scales and diverse material arrangements, has driven the adoption of numerical methods such as homogenization-based multiscale and global-local approaches, primarily through the finite element method (FEM), for high-fidelity micromechanical analysis of SiSC. A pioneering application of global-local methods in SiSC was made by Paggi et al. [15], focusing on intergranular failure in polycrystalline Silicon and leveraging specific scale separation under external mechanical loading.

Thus, the current study aims to develop a global-local phase field approach with solid shell elements to model cracks in solar cells within PV modules, emphasizing

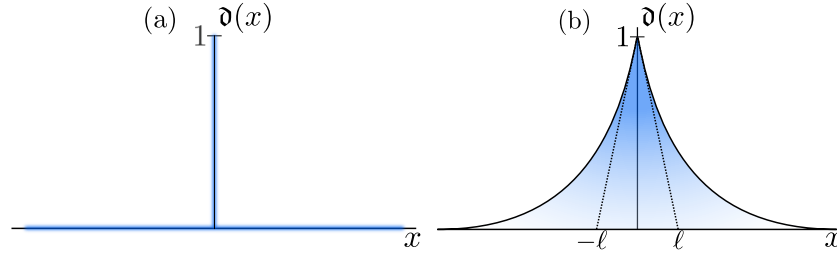


Fig. 1. Sharp (a) and diffusive (b) crack morphologies.

fracture modeling efficiency and capability. Fracture anisotropy is incorporated into the modeling to replicate crack patterns observed in experiments, demonstrating its relevance under various loading conditions.

2 Formulation

2.1 Phase-Field (PF) for fracture

The phase-field (PF) method for fracture is rooted in Griffith's theory [16], which postulates a competition between the elastic strain energy density, Ψ , and the fracture energy, $\mathcal{G}_C$. According to this theory, crack growth is governed by an exchange of energy: the formation of new crack surfaces increases the fracture energy while simultaneously reducing the elastic strain energy. Therefore, the framework establishes that a crack propagates when the reduction of elastic energy is more or equal to the increase in crack energy. The latter parameter is referred to $\mathcal{G}$, where $\mathcal{G}_C$ is the critical crack energy value, also called fracture toughness. Mathematically, this energy interplay is expressed through the global potential of the system, Π :

$$\Pi(\varepsilon) = \underbrace{\int_{\Omega/\Gamma} \Psi \, dV + \int_{\Gamma} \mathcal{G}_C \, dA}_{\Pi_{\text{int}}} - \Pi_{\text{ext}} \quad (1)$$

being ε the symmetric strain tensor; Ω , the volume domain; and Γ , a discrete internal discontinuity within the body.

The contribution to the internal functional rendering of the energy dissipation due to fracture events is recalled through the PF approach of fracture postulated by Francfort and Marigo [17]. Such variation framework replaces the concept of a sharp crack with a diffuse region ranging from pristine ($\mathfrak{d} = 0$) to damaged material ($\mathfrak{d} = 1$), see Fig. 1. From this, finding a global minimum in the potential of the Griffith's equation (Eq. (1)) is the main mission for the PF method. Thus, the regularization of the crack functional in the solid is performed as:

$$\int_{\Gamma} \mathcal{G}_C \, dA \approx \int_{\Omega} \mathcal{G}_C \mathcal{H}(\mathfrak{d}, \nabla \mathfrak{d}) \, dV \quad (2)$$

$\gamma(\mathfrak{d}, \nabla \mathfrak{d})$ denotes the crack surface density function, which follows a Poisson-type equation as:

$$\int_{\Omega} \gamma(\mathfrak{d}, \nabla \mathfrak{d}) \, dV = \int_{\Omega} \frac{1}{c_w} \left[\frac{1}{\ell} w(\mathfrak{d}) + \ell |\nabla \mathfrak{d}|^2 \right] \, dV \quad (3)$$

where the length scale parameter ℓ reflects the width of the smearing function, meaning that $\ell \rightarrow 0$ approximates the sharp crack topology. In addition, $w(\mathfrak{d})$ is the crack distribution according to the PF parameter and c_w is the scaling parameter. For our specific PF formulation, we follow the AT-2 approach postulated by Bourdin et al. [18], that states $c_w = 2$ and $w(\mathfrak{d}) = \mathfrak{d}^2$. Therefore, this variational formulation proposes the following value for γ

$$\int_{\Omega} \gamma(\mathfrak{d}, \nabla \mathfrak{d}) \, dV = \int_{\Omega} \frac{1}{2\ell} \mathfrak{d}^2 + \frac{\ell}{2} |\nabla \mathfrak{d}|^2 \, dV \quad (4)$$

Recalling the previous derivations, the crack can be regularised by this transition region, and therefore, the potential strain energy function expressed in Eq. (1) can be rewritten as:

$$\Pi(\varepsilon, \mathfrak{d}) = \int_{\Omega} g(\mathfrak{d}) \Psi(\varepsilon) \, dV + \int_{\Omega} \mathcal{G}_C \gamma(\mathfrak{d}, \nabla \mathfrak{d}) \, dV - \Pi_{\text{ext}} \quad (5)$$

where $g(\mathfrak{d})$ is the degradation function and its role is to reduce the elastic strength of the material upon crack propagation. For AT-2, the degradation functions reads as $g(\mathfrak{d}) = (1 - \mathfrak{d})^2 + \mathcal{K}$, where $\mathcal{K}$ is a small parameter used to avoid ill-conditioning in the stiffness matrix upon broken stage.

2.2 Shear locking

The problem of shear locking affects the compliance of the specimen when bending loads are applied on the specimen. In order to overcome this shear locking pathology, we combine the low-order displacement FE interpolation with the EAS method.

This method consists in the enhancement of the displacement-derived symmetric strain tensor ε'' by considering an incompatible strain tensor $\tilde{\varepsilon}$, which leads to an additive decomposition of such tensor as $\varepsilon = \varepsilon'' + \tilde{\varepsilon}$, following [20], where is performed for large deformations on the Green-Lagrange strain tensor.

Considering the orthogonality condition with respect to the stress field, the enhanced strains are interpolated at the element level using the operator $\mathbf{M}(\xi)$:

$$\tilde{\varepsilon} \approx \mathbf{M}(\xi) \cdot \varsigma, \quad \delta \tilde{\varepsilon} \approx \mathbf{M}(\xi) \cdot \delta \varsigma, \quad \Delta \tilde{\varepsilon} \approx \mathbf{M}(\xi) \cdot \Delta \varsigma \quad (6)$$

where ς are the stored incompatible strains on the nodal level. The operator $\mathbf{M}(\xi)$ can be calculated as:

$$\mathbf{M} = \frac{\det \mathbf{J}_0}{\det \mathbf{J}} \mathbf{T}_0^T \cdot \mathbf{M}_{\xi} \quad (7)$$

where $\mathbf{J}_0$ and $\mathbf{J}$ are the Jacobians, evaluated at the center of the element and at the Gauss integration point, respectively; $\mathbf{T}_0^T$ is the transpose of the inverse of a matrix that accounts for the terms of the Jacobian from the center that reads:

$$\mathbf{T}_0 = \begin{bmatrix} J_0^2_{11} & J_0^2_{21} & J_0^2_{31} & 2J_{011}J_{021} & 2J_{021}J_{031} & 2J_{011}J_{031} \\ J_0^2_{12} & J_0^2_{22} & J_0^2_{32} & 2J_{012}J_{022} & 2J_{022}J_{032} & 2J_{012}J_{032} \\ J_0^2_{13} & J_0^2_{23} & J_0^2_{33} & 2J_{013}J_{023} & 2J_{023}J_{033} & 2J_{013}J_{033} \\ J_{011}J_{012} & J_{021}J_{022} & J_{031}J_{032} & J_{011}J_{012} + J_{021}J_{012} & J_{021}J_{032} + J_{031}J_{022} & J_{011}J_{032} + J_{031}J_{012} \\ J_{012}J_{013} & J_{022}J_{023} & J_{032}J_{033} & J_{012}J_{023} + J_{022}J_{013} & J_{022}J_{033} + J_{032}J_{023} & J_{012}J_{033} + J_{033}J_{013} \\ J_{011}J_{013} & J_{021}J_{023} & J_{031}J_{033} & J_{011}J_{023} + J_{021}J_{013} & J_{021}J_{033} + J_{031}J_{023} & J_{011}J_{033} + J_{031}J_{013} \end{bmatrix} \quad (8)$$

Without any loss of generality, we recall the incompatible strain modes defined in [21] encompassing 24 incompatible modes for the matrix $\mathbf{M}_\xi$:

$$\mathbf{M}_\xi = \begin{bmatrix} \xi & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\eta & \xi\zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & \eta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\eta & \eta\zeta & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & \zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\zeta & \eta\zeta & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \xi & \eta & 0 & 0 & 0 & 0 & \xi\zeta & \eta\zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi\eta & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & \xi & \zeta & 0 & 0 & 0 & 0 & \xi\eta & \zeta\eta & 0 & 0 & 0 & 0 & 0 & 0 & \xi\zeta \\ 0 & 0 & 0 & 0 & 0 & \eta & \zeta & 0 & 0 & 0 & \xi\eta & \xi\zeta & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & \eta\zeta & 0 \end{bmatrix} \quad (9)$$

2.3 Material laws

The comprised materials in this work follow an elastic strain energy density which is defined as a function of the elastic strains and a linear elastic stiffness matrix $\mathbb{C}_0$ in the usual manner

$$\Psi(\boldsymbol{\varepsilon}) = \frac{1}{2}(\boldsymbol{\varepsilon})^T : \mathbb{C} : \boldsymbol{\varepsilon} \quad (10)$$

We have employed two different approaches in this framework. While it is true that Silicon follows a linear anisotropic behavior due to its polycrystalline behavior, see [10], we have included as well an isotropic approach for comparison where $\mathbb{C}$ can be easily obtained from the Hooke's law:

$$\mathbb{C}_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ik} \delta_{jl} + \delta_{il} \delta_{jk}) \quad (11)$$

where λ and μ are the Lamé constants. For the anisotropic case, the formulation is more complex: we know that $\sigma_{ij}^{\text{global}} = \mathbb{C}_{ijkl}^{\text{global}} \epsilon_{kl}^{\text{global}}$. However, since we are working on polycrystalline Silicon, we will have various grain distributions and orientations. Therefore, we will have to refer to a local state of the specimen. From [10], we define the following local linear elastic stiffness matrix, due to its cubic symmetry:

$$\mathbb{C}_{ijkl}^{\text{local}} = \begin{bmatrix} \mathbb{C}_{11} & \mathbb{C}_{12} & \mathbb{C}_{12} & 0 & 0 & 0 \\ \mathbb{C}_{12} & \mathbb{C}_{11} & \mathbb{C}_{12} & 0 & 0 & 0 \\ \mathbb{C}_{12} & \mathbb{C}_{12} & \mathbb{C}_{11} & 0 & 0 & 0 \\ 0 & 0 & 0 & \mathbb{C}_{44} & 0 & 0 \\ 0 & 0 & 0 & 0 & \mathbb{C}_{44} & 0 \\ 0 & 0 & 0 & 0 & 0 & \mathbb{C}_{44} \end{bmatrix} \quad (12)$$

In this material frame, the stress-strain relation can be symbolically written as $\sigma_{ij}^{\text{local}} = \mathbb{C}_{ijkl}^{\text{local}} \epsilon_{kl}^{\text{local}}$. For the particular case of Silicon, we have $\mathbb{C}_{11} = 165.7$ GPa, $\mathbb{C}_{12} = 63.9$ GPa and $\mathbb{C}_{44} = 79.6$ GPa. To effectively consider the material properties in a global setting, we use the three Euler angles defining the intersection (from Miller's indices a , b and c) between the surface plane $[abc]$ of the grain defined by its normal vector $\langle abc \rangle$ and the basic symmetry planes $[100]$, $[010]$ and $[001]$. Those angles are obtained as:

$$\theta_{100} = \arccos\left(\frac{a}{\sqrt{a^2 + b^2 + c^2}}\right) \quad (13)$$

$$\theta_{010} = \arccos\left(\frac{b}{\sqrt{a^2 + b^2 + c^2}}\right) \quad (14)$$

$$\theta_{001} = \arccos\left(\frac{c}{\sqrt{a^2 + b^2 + c^2}}\right) \quad (15)$$

Thus, the stress-strain constitutive relation for each arbitrarily oriented grain in the global reference systems reads $\sigma_{ij}^{\text{global}} = \mathbb{C}_{ijkl}^{\text{global}} \epsilon_{kl}^{\text{global}}$, where $\mathbb{C}_{ijkl}^{\text{global}} = R_{pi} R_{qj} R_{kr} R_{ls} \mathbb{C}_{pqrs}^{\text{local}}$. The rotation matrix $\mathbf{R}$ appearing in this transformation formula can be computed as follows $\mathbf{R} = \mathbf{R}_{001} \mathbf{R}_{010} \mathbf{R}_{100}$, whose terms are defined as follows:

$$\mathbf{R}_{100} = \begin{bmatrix} 1 & 0 & 0 \\ 0 \cos(\theta_{100}) & -\sin(\theta_{100}) \\ 0 \sin(\theta_{100}) & \cos(\theta_{100}) \end{bmatrix} \quad (16)$$

$$\mathbf{R}_{010} = \begin{bmatrix} \cos(\theta_{010}) & 0 & \sin(\theta_{010}) \\ 0 & 1 & 0 \\ -\sin(\theta_{010}) & 0 & \cos(\theta_{010}) \end{bmatrix} \quad (17)$$

$$\mathbf{R}_{001} = \begin{bmatrix} \cos(\theta_{001}) & -\sin(\theta_{001}) & 0 \\ \sin(\theta_{001}) & \cos(\theta_{001}) & 0 \\ 0 & 0 & 1 \end{bmatrix} \quad (18)$$

For this work, we are considering grains with crystallographic planes whose Miller's indices for the normal are $\langle 100 \rangle$, $\langle 110 \rangle$ and $\langle 111 \rangle$, which represent the vast majority of identified planes on Silicon polycrystalline structures.

2.4 Global-Local methodology

The submodeling technique is a computational approach to capture different length scales. Multilevel global-local methods rely on the type of information transfer and the relation between the different models throughout the analysis. In the related literature, the following categories are often used: (i) One-way coupling and two-way coupling (regarding the direction of the information transfer) (ii) Loose coupling and tight coupling (referring to the type of the information transfer) and (iii) Pointwise coupling and volume wise coupling (regarding the proportion between the models).

In this study, the global and local models are solved sequentially. First, the global model is solved and then, its results are applied as boundary conditions to the local

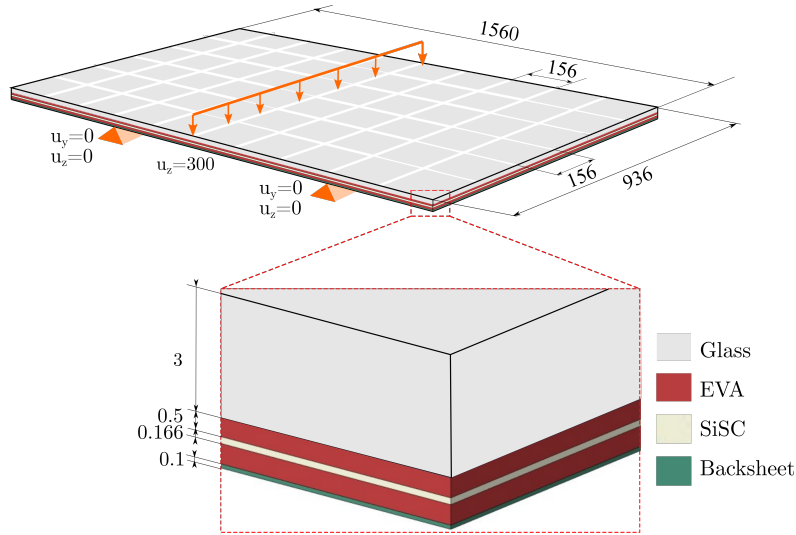


Fig. 2. Photovoltaic panel subject to bending load, showing the overall dimensions [mm] of the global specimen along with its boundary conditions. A zoom-in is performed along the thickness direction to provide detailed information on the size and distribution of the various layers within the solar panel. Local computations are carried out on a sub-cell of the SiSC layer, located at the center of the specimen. The sub-cells are clearly delineated by the white squares plotted.

model. This setup uses a one-way coupling, where degrees of freedom (DOFs) are transferred between the different levels in a single direction, along with a loose coupling approach in which both models are solved separately in sequential computations.

Generally, a global finite element model with coarse mesh is used to compute the displacement field in the global model, identifying the size and location of the critical regions with a low computational cost. Subsequently, the displacements output from global model are interpolated to set the boundary conditions for the local model, which represents a more detailed fine-scale of the critical area to achieve a higher accuracy.

3 Problem: photovoltaic panel under bending load

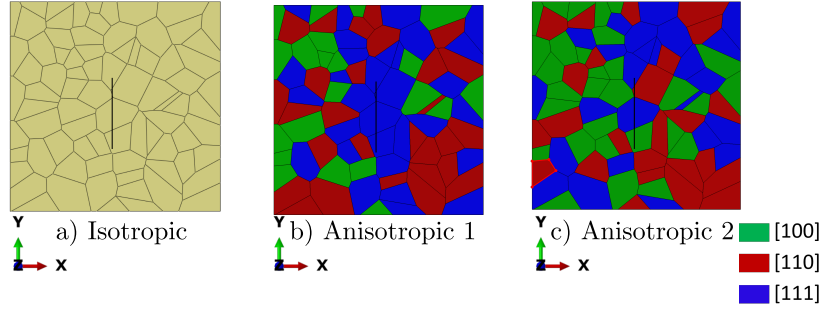
In this section, the global-local approach for phase-field fracture modeling is evaluated through solar panel cell cracking within a photovoltaic (PV) module subjected to three-point bending.

Fig. 3 illustrates the specimen's dimensions in millimeters, with a zoomed-in view revealing the layered structure of the PV panel. The material properties of this PV panel are specified in Table 1. The panel is subjected to a bending load by applying a displacement of $u_z = 300$ mm at the center of the sample.

The study begins by applying a bending load to the global specimen. Following this, a focused local analysis is conducted on a cell (highlighted by white squares) positioned at the center of the SiSC panel. For this localized investigation, we examine

Table 1. Properties for the solar panel, here encompassing the layers of glass, EVA and backsheet.

Material	E (GPa)	ν
Glass	68.95	0.23
EVA	7.90	0.411
Backsheet	3.58	0.271

**Fig. 3.** Three different cells analyzed. From left to right, we read: a) isotropic material for reference and b)-c) anisotropic cell resembling a polycrystalline Silicon with random grain orientations (caption referred to the Miller's indices of each grain).

three distinct PV sub modules, each one comprising 60 cells, with displacements interpolated from the global model to define the local boundary conditions. These conditions are updated at each time step to maintain fidelity in capturing the cell's mechanical response. A high-resolution mesh, composed of 200,092 C3D8 elements, is used for the local Silicon cells.

The three distinct PV modules analyzed are highlighted in Figs. 3(a)-c). To achieve a localized crack profile, a notch nucleating from the centre is introduced with a length equal to one-third of the subcell's width. In the first probe, studied only for reference, we use an isotropic model, defined by a Young's modulus of $E = 210$ GPa and a Poisson's ratio of $\nu = 0.3$. The remaining two specimens, however, are anisotropic samples with varied grain orientations to mimic the polycrystalline Silicon structure typical in PV cells. Using the specified properties for Silicon detailed in Sec. 2.3, we assign different grain orientations, as illustrated in the captions of Figs. 3(b)-c), where we provide the Miller indices for each grain orientation. This approach facilitates a more realistic representation of the mechanical behavior in polycrystalline PV cells under loading conditions.

The main results are illustrated in Figs. 4(a)-(c), which show the evolution of the crack for different bending loads across each of the three polycrystalline Silicon sub-modules. These micrographs use the phase-field parameter to visualize crack evolution, enabling a comprehensive comparison of fracture patterns across distinct loading conditions and grain orientations in each sub-module. For the isotropic specimen, shown in Fig. 4(a), we observe crack nucleation at a displacement of $u_z = 90$ mm, with slight deviation resulting from the bending characteristics. As the displacement increases, the

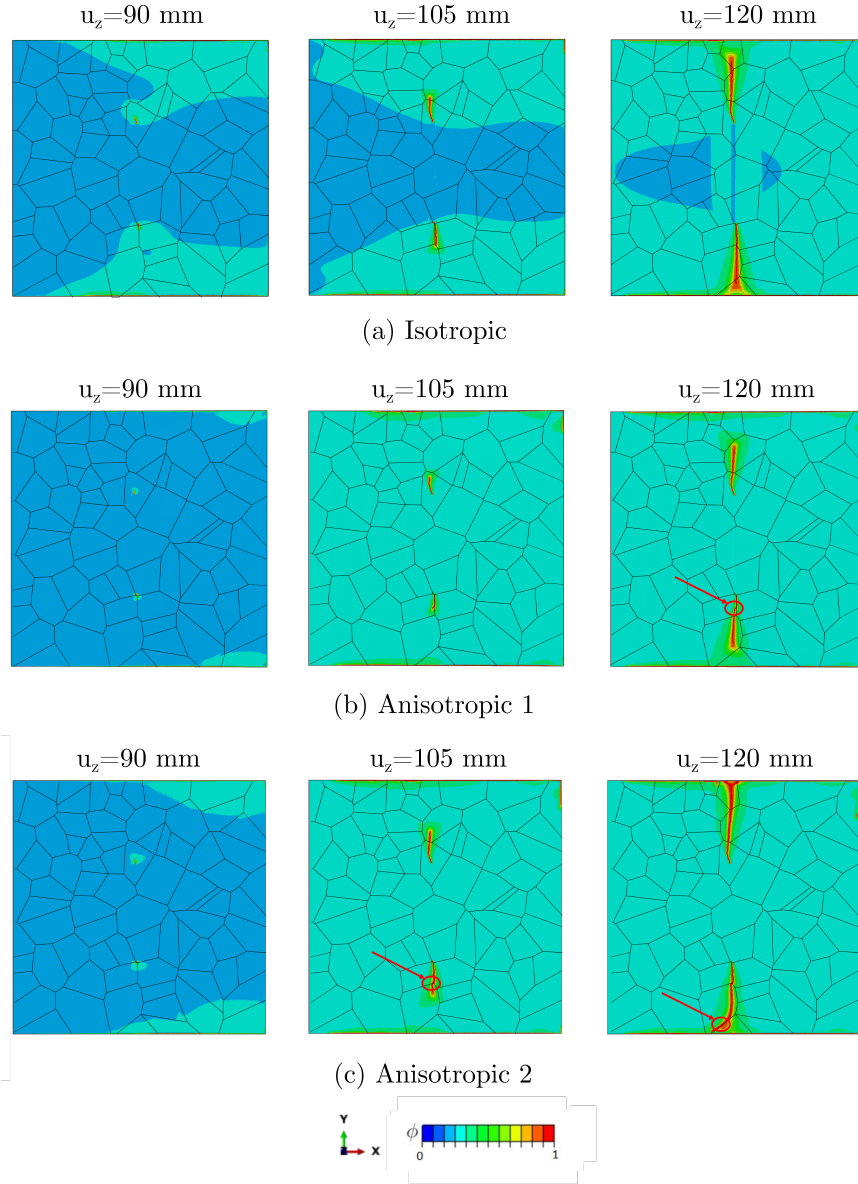


Fig. 4. Evolution of the crack propagation profiles for the (a) isotropic, (b) first anisotropic and (c) second anisotropic scenarios for the solar panel cell. Plotted is the phase field parameter isocontours with the legend case, where blue and red denote intact and broken states, respectively.

crack trajectory remains undeviating, which is typical behavior for an isotropic material. However, for the anisotropic specimens, the scenarios completely change. For the first anisotropic specimen (Fig. 4(b)) at a displacement of $u_z = 120$ mm and the second

anisotropic specimen (Fig. 4(c)) at $u_z = 105$ mm, deflections of the crack are observed at the grain boundaries (highlighted by a red circle), at the intersections of grains with different orientations (as depicted by the Miller's indices in Figs. 3b)-c)). Additionally, a second crack deviation occurs in the second anisotropic specimen at $u_z = 120$ mm as the crack approaches the bottom end of the sample. Such observed deflections during crack propagation is indicative of the interplay between intergranular and transgranular fracture mechanisms at the microscopic level, a phenomenon commonly observed in polycrystalline materials [10, 22]. These findings demonstrate the capability of our model to capture the complex crack propagation patterns that may emerge in polycrystalline Silicon PV modules under bending loads.

4 Conclusions and future developments

A global-local finite element model has been developed to analyze fracture behavior in Silicon photovoltaic panels at the granular level. Our preliminary results show that this approach manages to capture the crack initiation and propagation in (anisotropic) polycrystalline Silicon within solar cells, providing insights of failure mechanisms without the high computational cost that fully detailed models require.

Future developments for this research will include addressing key factors such as the grain size and boundary effects under static loading conditions to achieve greater accuracy in crack behavior prediction. Additionally, the study will be extended to analyze dynamic conditions, including fatigue and impact scenarios, to evaluate the durability and long-term performance of photovoltaic panels under more realistic scenarios. Finally, the model will be extended for ductile fracture analysis in perovskite-based photovoltaic panels, addressing the unique mechanical properties of this advanced solar technology.

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