A three dimensional concurrently coupled adaptive multiscale method for fracture

Pattabhi Budarapu1*, José Reinoso2, Marco Paggi1

1IMT Institute for Advanced Studies
19 Piazza Sanfrancesco
55100 Lucca, Italy
pattabhi.budarapu@imtlucca.it, marco.paggi@imtlucca.it

2Elasticity and Strength of Materials Group, School of Engineering
University of Seville, Camino de los Descubrimientos s/n
41092 Seville, Spain
jreinoso@us.es

ABSTRACT

Silicon (Si) is a non-toxic, abundantly available resource, having a broad spectrum absorption range of solar radiation. In the last decades, Silicon has been extensively used in the computer industry as well as other industrial sectors to produce electronic and renewable energy devices, among other. This is the case for instance of photo-voltaic applications, where it has been incorporated in the form of thin cells. However, from the mechanical point of view, due to the brittle nature of Silicon, defects are bound to happen during the manufacturing, transportation, installation and operation. The presence of such defects can initiate the micro-cracks, which can significantly affect the cell performance [1]. Experimental verification of the fracture properties of Silicon is difficult due to the practical difficulties in setting up the suitable experimental programs for this purpose. On the other hand, with the aim of overcoming these limitations, molecular dynamics (MD) simulations promise to accurately estimate the fracture properties of Silicon. However, due to nano-scale dimensions of atoms, pure MD simulations are computationally expensive with the current numerical capabilities. Therefore, multiscale methods are required to couple the continuum description of the structure with an atomistic description [2].

In the current contribution, we present a three dimensional concurrently coupled adaptive multiscale method (3DAMM) method to investigate the crack growth based on the minimum energy criteria. First, a molecular statics model is used near the crack tip. Cracks in the atomistic domain are modeled by restricting the neighbour interactions. To ensure self-consistency in the bulk, a nonlinear solid shell finite element [3] is used to model the material of the coarse scale continuum. This solid shell formulation is here employed due to the bending dominated deformations patterns in thin solar cells. Cracks in the continuum are incorporated based on the phantom node method. The coupling between the coarse scale and fine scale is realized through ghost atoms. The ghost atom positions are interpolated from the continuum solution and enforced as the boundary conditions on the fine scale. The fine scale region is adaptively enlarged as the crack propagates and the model behind the crack tip is adaptively coarsened [4]. Atoms on the crack surface are identified based on the centro symmetry parameter (CSP). The proposed modeling strategy is applied to study the fracture in Silicon.

References