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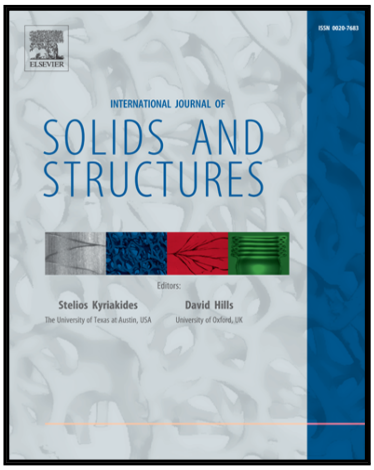

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Abstract

Polymer oxidation is a major degradation mechanism in organic solar cells. However, microstructural details of diffusion-reaction processes and oxidation-induced failure in structured semi-crystalline active layers are difficult to be predicted or measured, due to material heterogeneities, such as different material phases, crystallinities, nano-film thickness. Hence, a diffusion-reaction process has been coupled to a crystalline-amorphous material model and fracture algorithm within a nonlinear microstructurally-based finite element (FEM) framework to investigate and predict heterogeneous oxidative degradation and embrittlement failure in semi-crystalline organic thin films due to the interrelated effects of diffusion, reaction, stress accumulations, and crystalline packing order. The edge-on packing oriented film was more susceptible to oxidation than the face-on oriented packing film due to higher local stresses and reaction accumulations that resulted in higher decrease of local toughness and extensive film cracking in the amorphous phase. The coupled effects of mechanical stresses and oxygen diffusion-reaction accelerated degradation mechanisms and resulted in film cracking and delamination occurring at lower nominal strains in comparison with the case without oxidation embrittlement. Degradation was dominated by the reaction process and exposure time, as opposed to the diffusion process due to the nano-sized