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Parametrically Homogenized Constitutive Models (PHCM) from Image-based Crystal Plasticity Modeling to Predict Fatigue Crack Nucleation

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In this paper, an image-based concurrent multi-scale modeling framework is developed for predicting fatigue crack initiation in structures of titanium alloys, e.g. Ti7Al and Ti 6242. To enable the material-structure connection, this work develops parametrically homogenized continuum models (PHCM) from rigorous crystal plasticity analysis of statistically equivalent RVE's of the polycrystalline materials microstructure that includes models of crack initiation. Parametrically homogenized constitutive models (PHCMs) are reduced order continuum models for which constitutive parameters and their evolution are expressed in terms of statistical distribution functions of morphological and crystallographic parameters. Machine learning concepts can be used in determining the functional forms of the dependencies. PHCMs are many orders of magnitude more efficient than pure micromechanical analyses with comparable accuracy. The general forms of the PHCMs represent fundamental requirements, e.g. anisotropy, tension-compression asymmetry, history/path-dependence, objectivity, etc. that are expected in the material's macroscopic response. A strong point of departure of PHCMs from conventional phenomenological models is in the manifestation of constitutive parameters and their dependencies. Unlike those developed from experiments, these models are designed to have explicit dependence on the microstructural variables of morphology, crystallography etc., through functions that represent their aggregated distributions. In addition, these constitutive parameters also evolve with macroscopic state variables that manifest aggregate effects of the microstructural deformation mechanisms.

In addition to the PHCMS, a parametrically homogenized fatigue crack nucleation model is developed to predict crack initiation in macroscopic simulations using the concurrent multiscale simulation framework and machine learning methods. Multi-scale simulations predict that majority of cracks initiate sub-surface, which is in agreement with X-ray computed tomography observations. An image-based multi-scale modeling approach is essential in predicting localization and fatigue failure in structural components, since the governing aspects of the problem span different length scales: (i) local crystallographic microstructure, (ii) millimeter-scale material heterogeneities and (iii) structural-scale boundary conditions simultaneously play role in fatigue crack formation and growth.

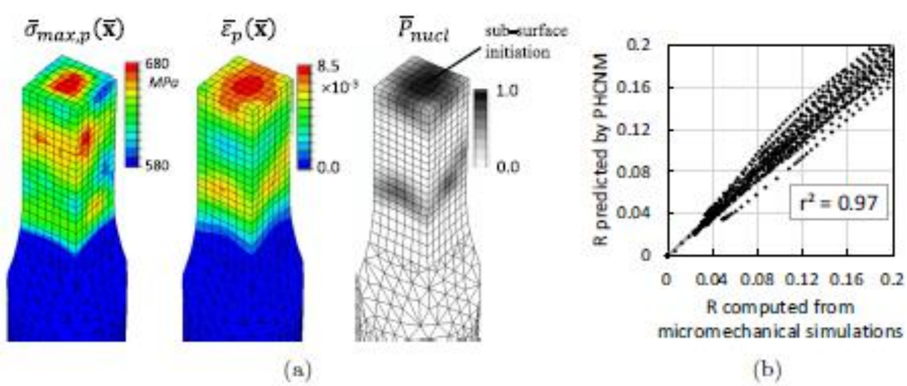

Figure 1. (a) Macroscopic PHCM-based FE simulations of a test specimen showing contour plots of maximum principal stress, effective plastic strain and the PHCNM-based crack nucleation probability distribution; (b) comparison of macroscopic crack nucleation variable R predicted by PHCNM and computed by 20 micromechanical CPFE simulations..

References

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