8th. World Congress on Computational Mechanics (WCCM8)
5th European Congress on Computational Methods in Applied Sciences and Engineeering (ECCOMAS 2008)
June 30 –July 5, 2008
Venice, Italy

APPLICATION OF AN ATOM CONTINUUM MODEL IN PROCESS OF DAMAGE SIMULATION ON MULTIPLE LENGTH SCALES

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Key Words: *Hierarchical Multiscale Concept, Polycrystal Model, Atom Continuum Model, Damage Analysis.*

ABSTRACT

The damage evolution in technical materials is a process that simultaneously proceeds on multiple length scales. Based on this knowledge the crack initiation and propagation as source of damage progress can be investigated in detail following a multiscale strategy. Therefor, we propose a hierarchical multiscale concept that transfers successively damage information from representative volume elements (RVE's) on lower scales to new material models on higher scales. Figure 1 illustrates the length definition of the micro, meso and macro scale in our concept. The current research is focused on metallic polycrystalline materials and, especially, crack growth along grain boundaries is investigated as the main source of damage evolution in these materials.

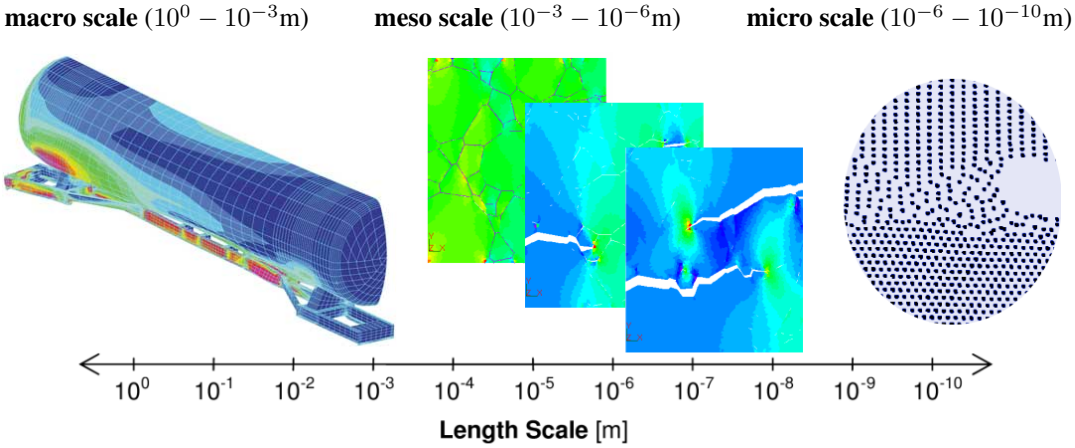

Figure 1: Multiple length scales are defined to investigate the damage evolution in a multiscale process.

In order to take into account that the physical process of damage starts on micro scale we investigate the atomic debonding along grain boundaries by application of an atom continuum model. The atom

continuum model is based on the idea of representative atoms that was introduced by Tadmor et al. [1] in the course of the quasicontinuum method. Based on atomistic energy laws, this method allows a reproduction of atomic debonding as the source of micro crack initiation in zones of localized damage. In undamaged model regions conventional continuum mechanical formulations are applied to calculate the structural response. During the simulation, zones of atomistic resolution are adapted following the progress of damage. Therewith, the method allows a significant reduction of degrees of freedom compared to pure atomistic methods and ensures a high accuracy on the atomic level at the same time. After the first version of the quasicontinuum method was limited to quasistatic calculations at zero temperature, some further developments were proposed to extend the method either to finite temperature [2] or to include the dynamics of the atoms [3]. Our three dimensional atom continuum model combines the dynamics of the atoms and application at finite temperature with the aim of a more realistic calculation of atomic debonding along grain boundaries on the micro scale.

On the meso scale we analyse the damage evolution along grain boundaries by using a polycrystal model, wherein the polycrystalline material structure is described by a three dimensional Voronoi cell diagram. Therein, each cell represents a single crystal and an orthotropic linear elastic material model is assigned to the crystals. In the analysis both, crystal orientation and material properties of each crystal are distributed by stochastic fields. The grain boundary decohesion process on the meso scale in the form of crack initiation and propagation is simulated by using a coupled cohesive zone model (CCZM) that is applied in the interfaces between single crystals. In the CCZM the peak strength depends directly on the missorientation between neighbouring crystals. Previous publications [4,5] show the application of the polycrystal model to analyse the crack initiation and propagation in statically loaded three dimensional RVE's of aluminium on the meso scale without necessity of any initial damage definition. In a further development the currently used CCZM of the meso scale model shall be substituted by an improved interface law that is derived from homogenized atom continuum simulation on the micro scale. A nontrivial problem concerning the homogenization has to be solved for the non-periodic damage situation in the micro scale RVE. Therefor, the classical approaches of homogenization cannot be applied and new algorithms are necessary.

In the future work it is planed to capture the accumulating damage on macro scale by an anisotropic damage tensor. Following the concept of hierarchical multiscale models the parameters of the damage tensor shall be evaluated by homogenization on RVE's of the polycrystal model on meso scale.

Acknowledgement: This research is supported by the German Research Council (DFG), which is gratefully acknowledged by the authors.

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