Bridging the scales in fracture and damage mechanics

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On the engineering scale, continuum mechanics provides an efficient way to model brittle fracture based on stresses, stress intensity factors, and energy release rates. On the atomic scale, in contrast, brittle fracture occurs by the breaking of atomic bonds, which is caused by exceedingly high interatomic forces. To describe ductile failure in metals, typically damage models are employed that mimic the physical process of nucleation, growth and coalescence of voids that is driven by plastic deformation and small-scale diffusion of monoatomic vacancies. In both, brittle fracture and ductile failure, the microstructure of the material plays a dominant role to determine the failure mechanism and the loading conditions at which failure occurs. Hence, it is seen that a comprehensive understanding and a consistent description of brittle fracture and ductile failure involves a number of length and time scales. The length scales are ranging from the atomic over the microstructural to the component scale, thus, covering roughly nine orders of magnitude; the involved time scales range from atomic oscillations to diffusive times, which poses and even more severe scale bridging problem, as more than twelve orders of magnitude need to be considered. To accomplish this, scaling methods are required that allow for the transfer of fundamental atomistic information and knowledge about the mechanisms occurring within the microstructure to models that solve engineering problems.

In this lecture, focusing on the implications of bridging several length scales, an overview is provided on methods that are used to describe damage and fracture on the macroscale, i.e. cohesive zone models for brittle and semi-brittle fracture and damage models for ductile failure. In a top-down scale bridging approach, these engineering models are augmented with information on atomic and microstructural processes, to capture the essence of the physical mechanisms occurring on the relevant length scales. In this way, atomistically and microstructurally informed continuum models are introduced and examples for their applications are given. In these applications, atomistically informed cohesive zone models for fracture in brittle ceramics with a heterogeneous microstructure are discussed [3], together with a physically motivated scaling scheme to transfer atomistic data into continuum fracture models [2]. Ductile failure models are introduced on the microstructural scale [1] and ways of homogenizing the material's damage behavior to the macroscale are revealed [4].

References

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