Structure-property modelling of the mechanics of materials across length scales

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In the past decades, considerable progress had been made in bridging the mechanical engineering aspects of materials to the field of materials science. This is mainly due to a fruitful combination of micromechanics and multi-scale approaches, with a steadily increasing multidisciplinary character. Several improved micromechanical theories and associated numerical models have been proposed and implemented, where a lot of interaction with materials science is involved. The developed understanding of single phases and complex interfaces in materials is optimally used in multi-scale homogenization techniques, where it is aimed to predict the collective multi-phase response of materials. Large deformations, damage and cracking, phase transformations, etc. can thereby be taken into account. This presentation focuses on this trend and illustrates some recent developments by means of a number of specific cases of interest.

At the microstructural scale, four examples will be given. The first example is a strain-gradient enriched crystal plasticity model for FCC metals, which takes into account the appearance of geometrically necessary dislocations and grain boundary dislocations at the grain level. Examples will be given to illustrate the influence of grain and/or specimen size upon mechanical loading. The second example concerns the integrity of solder joints in micro-electronics, where a microstructural evolution model for the occurring diffusion is combined with the mechanics of the phases. A classical Sn-Pb solder alloy is used to this purpose, where a nonlocal diffuse interface model inspired by the Cahn-Hilliard theory is implemented. Static failure within a Sn-Ag-Cu solder microstructure is described by a cohesive zone model, which accounts for the failure at the interfaces (phase or grain boundaries), which seems to be the dominating failure mechanisms encountered in practice. The third example briefly illustrates how the intrinsic relation between strain path effects in metals and dislocation substructures can be implemented in a simple micromechanical model. The last example concerns the quasi-brittle failure of a hard coating on a ductile substrate on the one hand, and the delamination of a soft polymeric coating from a metallic substrate on the other hand.

Each of these examples can be used within a multi-scale framework that aims to predict the macroscopic engineering response of materials in practical applications. The presentation closes by sketching some recent trends in multi-scale mechanics, where special attention is given to computational homogenisation schemes, which are based on the hierarchical solution of two coupled boundary value problems. Enriched computational homogenisation schemes permit to deal with localization and size effects in evolving materials. A short overview of such computational multi-scale models is given, with a special emphasis on their mutual links, on their inherent nonlocality and on the applicability to damage and localization.