

Micromechanics of deformation and fracture in highly cross-linked thermosets

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Advanced constitutive models for polymers have been essentially developed for thermoplastics with relatively limited applications/extensions to thermosets. Thermosets differ from thermoplastics by the cross-linking. Recent extensions of these constitutive models provide accurate predictions over a wide range of loading configurations, strain rates and temperature, encompassing below and above transition temperature regimes, although at the prize of a very large number of parameters, often larger than 30. Still, these models, mixing phenomenological and micromechanics ingredients, are often not rich enough to capture complex behaviors such as for instance severe non-linearity upon unloading, while missing also micromechanical connection to the failure process. Based on an extensive experimental test program on the highly cross-linked RTM6 epoxy, the viscoplastic response is found very similar to thermoplastics, with hardening-softening-re-hardening, large back stress upon unloading and existence of shear band patterns at very small scale. A molecular physics-based model of the deformation process occurring through the activation of nanometer scale shear transformation zones (STZ) has been developed, borrowed from the metallic glass field. The viscoplastic deformation is the result of the cooperative activation of STZ's, sensitive to rate, temperature, stress state and stress level. This model involves only 5 parameters to identify, all with physical meaning. The model quantitatively captures all the experimental trends, even some complicated responses during creep tests performed after plastic deformation at intermediate stress levels showing backward followed by forward creep. Such as model will never replace closed form constitutive models for the treatment of large scale components but can be used to understand small scale mechanics as well as for identifying macroscopic models. In this research, a new micromechanics-based fracture model based on the attainment of a local maximum principal stress within a given volume is also proposed and validated for a wide range of stress states.

Keywords: Micromechanics, viscoplasticity, fracture, polymers

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