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# FE prediction of microcracking in a 3D graphite polycrystal - evolution of the macroscopic response under temperature changes and irradiation

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## Abstract

The present study aims to predict the microscopic heterogeneity of stresses and strains inside a graphite polycrystalline aggregate. Graphite crystallites present a huge anisotropy in all regards: elastic stiffness, creep rates, thermal expansion and irradiation induced shape changes. As a result of the microscopic anisotropy, the cooperative (and geometrical compatible) deformation of adjacent crystallites in the bulk of a polycrystal induces high local stresses, which may trigger microcracking. The propagation of microcracks occurs both inside the crystallites (parallel to the basal planes) and along the grain boundaries. Once they are formed, microcracks are expected to decrease both the macroscopic Young modulus and the apparent coefficient of thermal expansion (CTE). They also affect the macroscopic creep rate. The phenomenon is simulated here using finite element modeling of a polycrystal made of Voronoi cells subjected periodic boundary conditions in 3D. Microcracking is accounted for by relying on user-defined cohesive-zone elements (UEL) whereas the response of individual graphite crystallites is computed based on a user-defined material law (UMAT). When compared to experimental trends, the predictions of the present model are shown to be more realistic than those obtained in a previous FEM study performed in 2D (1). (1) P. Yan et al., Carbon 96 (2016) 827-835

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