Coupled crystal plasticity and phase field modelling of intergranular failure of a heat-resistant steel during creep

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Abstract

A coupled crystal plasticity and phase field framework has been developed and applied to modelling intergranular failure of a heat-resistant steel during creep. The evolution of the order parameter (damage) was driven by both the elastic energy and a dislocation configuration stored energy that was derived from the crystal plasticity framework. The effect of intergranular carbide precipitates was incorporated by introducing a grain boundary characteristics dependent energy, resulting in a reduction in the local resistance to fracture of the grain boundaries. This approach enabled the prediction of local inelastic deformation fields and the distribution of phase field damage, providing a detailed evaluation of potential crack nucleation sites. The crystal plasticity model is calibrated and validated from the creep tests under various applied stress on an austenitic steel at 665°C. Predictions of creep deformation and creep rupture life are consistent with experimental data. After testing, different degrees of intergranular damage were observed in the specimens by scanning electron microscopy. Detailed grain boundary analyses using EBSD and TEM for the three different service time materials revealed that the primary mechanism responsible for creep damage initiation is the nucleation of microcavities at intergranular carbides. To further understand this mechanism, the contribution of different microstructural features was investigated through the simulations, including Schmid factor, dislocation densities, etc.

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