Crystal plasticity finite element modelling of coarse-grained α-Uranium

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ABSTRACT

α-Uranium, the stable phase of Uranium up to 670°C, has an orthorombic crystal structure. It exhibits complex deformation and fracture behaviour. Understanding the relationship between microstructure and mechanical properties is important to prevent fracture during manufacture and usage of components. The lattice of α-Uranium corresponds to a distorted close-packed-hexagonal crystal structure and it exhibits twins of both the 1st and 2nd kind. Therefore, undertaking detailed studies of the behaviour of α-Uranium can also contribute to the general understanding of the interaction between plasticity, twinning and fracture in crystals with high symmetry.

Plastic deformation in α-Uranium can be accommodated by 4 slip systems and 3 twin systems, previously identified by McCabe et al. [1]. These deformation modes are implemented into a crystal plasticity finite element (CPFE) solver. A temperature dependent, dislocation density based material model is developed to describe the critical resolved shear stress on the different slip/twin systems. The strong anisotropic thermal expansion behaviour is taken into account to simulate the development of internal residual stress states following casting of the material. During cooling, the internal stresses in α-Uranium are sufficient to induce plasticity. This effect is quantified using polycrystal simulations, in which first the temperature is decreased, then plastic relaxation takes place, followed by application of a mechanical load. The asymmetry between mechanical properties in tension and compression, due to the presence of twins, is investigated.

The model is calibrated using stress strain curves and the lattice strain found from neutron diffraction experiments carried out on textured samples at ISIS [2]. The slip/twin system strengths are found to be higher than in single crystal specimens, but lower than in fine-grained material. The CPFE method allows the heterogeneity of the strain between neighbouring grains and its influence on the evolution of the internal stress state to be investigated. This is a step forward compared to previous models that used the visco-plastic self-consistent (VPSC) method for this class of materials [3].

REFERENCES

[1] R.J. McCabe, L. Capolungo, P.E. Marshall, C.M. Cady, C.N. Tomé, *Deformation of wrought uranium: experiments and modelling*, Acta Materialia 58 (2010) 5447-5459.
[2] P. Earp, S. Kabra, J. Askew and T.J. Marrow, *Lattice strain and texture development in coarse-grained uranium – a neutron diffraction study*, (2018) J. Phys.: Conf. Ser. 1106, 012012.
[3] M. Zecevic, M. Knezevic, I.J. Beyerlein, R.J. McCabe, *Origin of texture development in orthorhombic uranium,* Materials Science & Engineering A 665 (2016) 108-124.