Venice, Italy

DEVELOPMENT OF A THREE DIMENSIONAL GRAIN STRUCTURE SUBMODEL FOR NUMERICAL MODELLING OF TI-6AL-4V AT ELEVATED STRAIN RATES

* Helen R. Sarsfield¹, Nik Petrinic²

Impact Engineering Team, Solid Mechanics and Materials Engineering Research Group, Department of Engineering Science, University of Oxford, Parks Road, Oxford, OX1 3PJ ¹helen.sarsfield@eng.ox.ac.uk ²nik.petrinic@eng.ox.ac.uk www.eng.ox.ac.uk

Key Words: Ti-6Al-4V, Microstructure, Reconstruction, Crystal plasticity

ABSTRACT

It is crucial that a material's response to the loading conditions to which it might be subjected in its lifetime can be accurately predicted. In order to characterise fully a material, its microstructure must be considered –the properties of titanium alloys are primarily determined by the morphology, volume fraction and individual properties of the two phases present [1]. This paper combines ideas from three disciplines *viz*. computational mechanics, experimental mechanics and materials science. It describes the development of a three dimensional Grain Submodel and outlines the role of crystal plasticity within the adopted strategy for characterization of a lightweight metallic alloy for aerospace applications subjected to impact loading, specifically the alloy Ti-6Al-4V.

The performance of Ti-6AL-4V has been investigated using uniaxial tensile tests over a range of strain rates from 1×10^{-3} to $1 \times 10^4 \text{s}^{-1}$. These data provide the boundary conditions for continuum finite element modelling and a nonlinear constitutive law was chosen for this, capable of representing the macroscopic behaviour of the rate dependent alloy [2]. Continuum micromechanics, in addition to material characterisation and constitutive modelling, can be used to study local phenomena in heterogeneous materials, such as the initiation and evolution of microscale damage and the nucleation and growth of cracks. One modelling strategy is to generate unit cells that follow as closely as possible the phase arrangement of a given sample, as obtained from metallographic sections. However, the actual modelling of complex phase configurations to a sufficient level of detail is extremely challenging. An alternative approach, presented here, is to generate a statistically geometrically representative grain structure model, a Grain Submodel.

This paper describes how microscopic observations, using electron back scattered diffraction, on two dimensional sections of the tensile specimens have been used to determine the phase arrangement and grain morphology of the material under investigation. A method has been developed to construct a three dimensional finite element model of the grain structure by analysis of the data from these two dimensional sections. The concept of a submodel which captures the microstructure of the material

will enable the macroscopic effects of changes in the microstructure to be investigated, and ultimately lead to the development of a framework for the design of a material to improve impact performance.

A micromechnical approach is developed to permit incorporation of an understanding of the deformation mechanisms at the crystalline level of the material into the predictive modelling capabilities: A crystal plasticity material model for explicit finite element analysis has been developed and implemented into a user defined material model in DEST (an in-house software package) [3]. This research contributes to a move away from the classical techniques, which are based on a phenomenological type of approach, towards a micromechanical one. This should lead to a better understanding of the processes occurring during deformation and allow us to optimise a material's performance by engineering its microstructure. The research was conducted in partnership with Rolls-Royce plc.

REFERENCES

- [1] Christoph Leyens and Manfred Peters, editors. *Titanium and Titanium Alloys: Fundamentals and Applications*, Wiley VCH, 2003.
- [2] H. Sarsfield, L. Wang, N. Petrinic. "An experimental investigation of rate dependent deformation and failure of three titanium alloys". *Journal of Materials Science*, Vol. 42, 5085-5093, 2007.
- [3] Nik Petrinic. *Aspects of discrete element modelling involving facet to facet contact detection and interaction*, PhD thesis, University of Swansea, 1996.