International Journal of Plasticity 61 (2014) 49–63

Contents lists available at ScienceDirect

International Journal of Plasticity

journal homepage: www.elsevier.com/locate/ijplas

Modelling the effect of elastic and plastic anisotropies on stresses at grain boundaries

D. Gonzalez [a,b], I. Simonovski [c], P.J. Withers [a], J. Quinta da Fonseca [a,*]

[a] School of Materials, University of Manchester, Grosvenor St., Manchester M13 9PL, UK
[b] Department of Engineering Science, University of Oxford, Parks Road, Oxford OX1 3PJ, UK
[c] Institute for Energy and Transport, P.O. Box 2, Petten NL-1755 ZG, The Netherlands

ARTICLE INFO

Article history:
Received 6 October 2012
Received in final revised form 10 March 2014
Available online 27 March 2014

Keywords:
A. Grain boundaries
B. Anisotropic material
B. Polycrystalline material
C. Finite elements
C. Boundary elements

ABSTRACT

It is believed that intergranular stresses play a significant role in failure processes, such as stress corrosion cracking (SCC) and fatigue cracking. In deformed cubic metals, intergranular stresses arise solely from the plastic and elastic anisotropies of the individual grains. In this work, stresses normal to the grain boundaries in deformed stainless steel have been calculated using crystal plasticity finite element modelling (CPFEM). The calculations show that, at strains larger than 0.5% and under load, the stress at grain boundaries is dominated by the effect of plastic anisotropy rather than elastic anisotropy. Upon unloading, plastic misfit still fully dominates the heterogeneity of normal stresses and is insensitive to the angle between the boundary normal and the preloaded direction. The effects of mesh density and size of boundaries on normal stresses are also studied. Special attention has been focused on examining what conditions give rise to large grain boundary stresses. Our results suggest that the magnitudes of the predicted residual grain boundary stresses are not highly correlated to the amount of plastic strain in the vicinity of the boundary and whether it is higher or lower than the average plastic strain. In other words, a soft-hard grain combination does not imply high tensile (nor compressive) residual stress normal to its boundary. The results are similar if instead of comparing the plastic strain near neighbours, we compare the plastic strain in the grain to the average plastic strain.

1. Introduction

Intergranular stresses are believed to be important for a range of grain boundary (GB) related failure mechanisms. For example, the brittle intergranular fracture of alumina can be related to the normal grain boundary stresses generated by the anisotropy in elastic constants (Aswad and Marrow, 2012; Gonzalez et al. 2013). Failure by stress corrosion cracking (SCC) in stainless steel often occurs intergranularly as illustrated in Fig. 1 by Babout et al. (2006). The reasons for this are complex, but, the magnitude of stress normal to the grain boundary is likely to be one of the contributing factors for intergranular cracking (Palumbo et al., 1991). Similarly, grain boundaries have been demonstrated to have an impact on the initiation of fatigue cracks in polycrystals (Sangid et al., 2011). In such cases, measuring the stresses at grain boundaries in the bulk is very difficult experimentally, if not altogether impossible, although some hope has recently raised with high resolution EBSD techniques (Gardner et al., 2010). Consequently, there is considerable interest in modelling deformation at the

* Corresponding author.
E-mail addresses: david.gonzalez@postgrad.manchester.ac.uk (D. Gonzalez), joao.fonseca@manchester.ac.uk (J. Quinta da Fonseca).

http://dx.doi.org/10.1016/j.ijplas.2014.03.012
0749-6419/

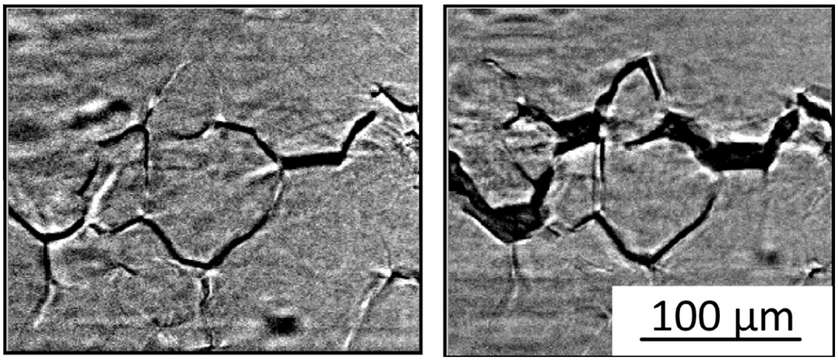

Fig. 1. Longitudinal sections from successive X-ray tomographs showing the same region in a sensitised type 302 stainless steel wire, demonstrating development of intergranular cracking (Babout et al., 2006).

grain scale and using these models to give estimates of local stresses at the microstructural level. At this scale, isotropic material models no longer apply and the inherent plastic and elastic anisotropy of crystals must be taken into account. One way of achieving this is to use effective-medium self-consistent models with appropriate single crystal plasticity laws. Such models can be used to successfully predict the evolution of the lattice strains during uniaxial tensile loading in stainless steels (Clausen et al., 1999) and to study the impact of single crystal elastic anisotropy on the lattice strains during the elastic–plastic transition (Clausen et al., 1998). Single crystal plasticity laws can also be incorporated into the finite element method (FEM) to model the deformation of polycrystals (Bate, 1999; Mika and Dawson, 1999; Delannay et al., 2006; Dunne et al., 2007a, 2012; McDowell and Dunne, 2010; Abdolvand et al., 2011). Further, crystal plasticity models have been used to predict the dislocation density across the boundary of a deformed aluminium bi-crystal (Liang and Dunne, 2009) as determined experimentally (Sun et al., 2000). The strengthening effect of grain boundaries has also been modelled using size-dependent constitutive laws (Lim et al., 2011; Ozdemir and Yalcinkaya, 2014). However, only in a few cases has crystal plasticity FEM been used to predict stresses right at the boundary (Diard et al., 2002, 2005; Kanjarla et al., 2010), perhaps due to the difficulty in measuring them.

In this article, we present the results of a systematic study on the development of normal stresses at grain boundaries during, and subsequent to, uniaxial deformation. The unloaded state is of particular interest due to the enhancing effect that prior deformation has on SCC and fatigue susceptibility (Mochizuki, 2007). Our study has two main aims: to determine the relative importance of elastic and plastic anisotropy on the development of grain boundary stresses and to determine whether the magnitude of the stresses can be correlated with the amount of plastic deformation in the grains that neighbour the boundary. In this respect, intergranular damage has been correlated to the deformation incompatibility (Bieler et al., 2009) and the amount of plastic strain in neighbouring grains (Couvant et al., 2009; McMurtrey et al., 2011; Scenini and Sherry, 2012; Stratulat et al., 2014). Here the emphasis is on the stresses acting normal to the grain boundaries, as these are probably the most relevant in the context of IGSCC.

In annealed metals, stresses at grain boundaries are likely to be relatively small, especially in those with a cubic crystal structure and which therefore have no thermal expansion anisotropy. When deformed, however, the magnitude of these stresses increases due to the mechanical anisotropy of individual grains. During uniaxial deformation, the magnitude of the stresses normal to the boundary depends on three major factors: boundary orientation with respect to the loading direction, elastic mismatches caused by the anisotropy single crystal elastic constants (Fallahi and Ataee, 2010) and plastic strain misfit caused by single crystal plastic anisotropy.

(1) *Boundary orientation with respect to the loading direction*. The resolved stress at the grain boundary depends strongly on the angle of the grain boundary plane with the loading direction.
(2) *Elastic mismatches caused by single crystal elastic anisotropy*. Most metals exhibit elastic anisotropy at the single crystal level. During deformation of a polycrystalline aggregate, this anisotropy causes the strain and stress within each grain to differ from their macroscopic average (Sauzay, 2007). As a consequence, deformation incompatibilities develop between neighbouring grains with different crystallographic orientations, giving rise to stresses at the grain boundaries. If deformation is purely elastic, these stresses disappear on unloading.
(3) *Misfit caused by plastic anisotropy*. If plastic deformation occurs by crystallographic slip, then the stress at which individual grains deform plastically will depend on the crystallographic orientation of the grains. Grain orientation will determine how many slip systems are activated and how easily they are activated in response to a given constraint. Some grains are therefore "harder" than average and others "softer" in certain directions. As in the elastic strain case, this plastic anisotropy leads to incompatibilities between neighbouring grains, with associated grain boundary stresses. The material discontinuity due to plastic anisotropy is maximum at the boundary relative to the center of the grains. As a consequence, stress variabilities are maximum at the boundary relative to the center of the grains, as found by Barbe et al. (2003) using CPFEM with only plastic anisotropies.