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A combined experimental-numerical approach for elasto-plastic fracture of individual grain boundaries ☆

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ABSTRACT

The parameters for a crystal plasticity finite element constitutive law were calibrated for the aluminum–lithium alloy 2198 using micro-column compression testing on single crystalline volumes. The calibrated material model was applied to simulations of micro-cantilever deflection tests designed for micro-fracture experiments on single grain boundaries. It was shown that the load–displacement response and the local deformation of the grains, which was measured by digital image correlation, were predicted by the simulations. The fracture properties of individual grain boundaries were then determined in terms of a traction–separation-law associated with a cohesive zone. This combination of experiments and crystal plasticity finite element simulations allows the investigation of the fracture behavior of individual grain boundaries in plastically deforming metals.

1. Introduction

Methods for investigations into the fracture properties of materials on a microscopic scale based on cantilever bending experiments (Di Maio and Roberts, 2005; Motz et al., 2005) were recently developed in order to gain a better understanding of the resistance of materials against damage and fracture. These experiments were focused on materials which show brittle failure like intermetallic compounds (Halford et al., 2005; Klüsner et al., 2011), interfaces in nano-components (Hirakata et al., 2007) and coatings (Di Maio and Roberts, 2005; Matoy et al., 2009). Moreover, small-scale experiments were conducted in order to isolate individual grain boundaries in technological materials (Armstrong et al., 2009, 2011). These experiments were carried out on materials that showed minor plastic deformation prior to fracture.

In general, plastic deformation limits the applicability of microscopic fracture experiments since the plastic zone in front of a crack tip tends to expand through the complete specimen leading to plastic deformation without fracture. However, plastic deformation prior to fracture was observed in recent microscopic fracture experiments. In a preliminary work, which was carried out on the aluminum lithium alloy 2198, grain boundaries were fractured after plastic deformation of the adjacent grains (Kupka and Lilleodden, 2012). This combination of ductile grains and brittle grain boundaries is an important case for ductile technological alloys that show intergranular fracture, e.g. aluminum–lithium alloys (Vasudevan and Doherty, 1987; Suresh et al., 1987). Recent micro-fracture experiments that were conducted on NiAl and tungsten single crystals also showed plastic deformation prior to fracture (Iqbal et al., 2012; Wurster et al., 2012) without the presence of a

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grain boundary. In these cases the anisotropic plastic deformation of the material surrounding the location of fracture must be taken into account for the fracture analysis.

Due to the complex boundary conditions associated with such experiments the analysis of the fracture properties is frequently carried out with the help of finite element simulations. For ductile specimens a suitable description of the plastic deformation is required. In the case of a grain boundary fracture experiments on the microstructural length scale the anisotropic plastic deformation of the grains must be taken into account. Within the framework of continuum mechanics the crystal plasticity finite element method (CPFEM) has evolved as a valuable tool to describe the anisotropic plastic deformation of textured materials and individual grains (Roters et al., 2010). For example, Raabe and Roters (2004) and Zhao et al. (2004) used a CPFEM model to predict the deformation of a textured component for a deep drawing process. Klusemann et al. (2012) determined the local deformation properties of oligo-crystalline tensile test specimens with the help of a CPFEM model. In these cases the CPFEM model provided a good prediction of the anisotropic plastic deformation of the material.

However, the identification of appropriate material parameters for a CPFEM model is not always straightforward. Especially in the case of technological materials, such as rolled sheets, bulk single crystal data is typically unavailable. One approach to circumvent this problem is to apply the micro-compression test developed by Uchic et al. (2004). Such tests have been successfully used to determine the deformation properties on a microscopic scale (Volkert and Lilleodden, 2006; Uchic et al., 2006; Greer et al., 2008). Raabe et al. (2007) used a calibrated CPFEM model to investigate the influence of the boundary conditions that are imposed in micro-compression experiments on the deformation behavior of single crystals. They numerically predicted the orientation evolution within micro-compression specimens and they showed the beneficial influence of the indenter to column friction. Furthermore, Soler et al. (2012) combined micro-compression experiments on single crystalline specimens with the CPFEM to investigate the deformation processes in LiF single crystals. They were able to show that a difference in the flow stress between different types of slip systems leads to an increased sensitivity against misalignments of the micro-column and the compression axis. Another approach for the parameter identification was pursued by Gong and Wilkinson (2009). They used micro-cantilever bending experiments on titanium single crystals as an experimental base for the parameter identification for a model created by Dunne et al. (2007) for hcp materials to identify the model parameters. These studies show that micro-mechanical experiments that are preferentially carried out on single crystalline volumes can provide access to the CPFEM parameters.

The purpose of the present work is to incorporate the anisotropic plastic deformation properties in terms of a CPFEM material model into the finite element based fracture analysis of a single grain boundary. While the CPFEM parameters are identified using micro-column compression experiments, the fracture analysis is performed using cohesive zone modeling of the grain boundary, which allows for a mechanism independent description of the fracture process.

2. Experiments

The experiments were conducted on the lithium containing aluminum alloy 2198 in the temper T351. The microstructure of the sheets of AA2198 consists of flat grains elongated in the primary rolling direction (see Fig. 1). The smallest dimension is the grain thickness, which is nominally 3 μm. The yield stress and the ultimate tensile stress for the material were determined by macroscopic tensile tests (see Table 1). For the simulations an elastic modulus of 75 GPa was assumed (Cavaliere and de Santis, 2008).

Both the cantilevers and the columns were fabricated using focused ion beam (FIB) milling (Nova200, FEI). The cantilevers were fabricated into the edge of the specimen, as given in Fig. 1. The approximate dimensions of the micro-columns and the micro-cantilevers in relation to the microstructure are also provided in Fig. 1. The geometry of the micro-cantilevers was adopted from a previous work (Kupka and Lilleodden, 2012). A micro-cantilever specimen is shown in

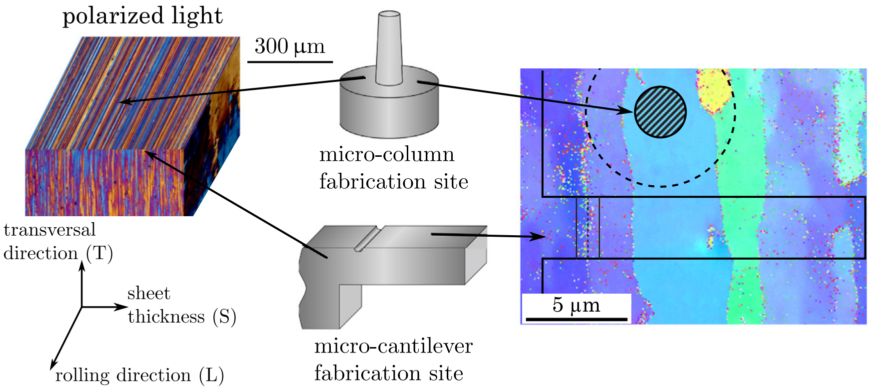

Fig. 1. The fabrication sites of the micro-columns and the micro-cantilevers in relation to the microstructure. The image in polarized light was recorded after Barker's etch (HBF_4+H_2O, anodized using 0.2 A/cm^2), the EBSD image was recorded from the polished surface.