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Orientation dependence of the fracture behavior of single-crystal tungsten

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Abstract

Polycrystalline tungsten at room temperature shows a brittle fracture behavior, which is also strongly influenced by the grain structure and texture as well as sample dimensions. To gain insight into the mechanical response of individual grains, an experimental program has been set up to test small scale samples under microbending starting with a notched tungsten single crystal oriented with the {110}<1$\bar{1}$0> crack system along the loading direction. Related to this experimental program a finite element study has been performed to analyze the crack propagation in such single-crystal tungsten micro cantilevers. The aim of the present numerical work is to investigate the influence of the single-crystal orientation on the fracture process.

A finite element (FE) model of the notched microbeam was created taking plastic deformation at the crack tip into account. Plastic deformation is implemented using a crystal plasticity approach formulated by Asaro (1983) and written by Huang (1991). Furthermore, the fracture process with crack propagation is described by a cohesive zone model. The simulations of microbending allow for evaluating the details of the fracture process more accurately. The results reveal details of the developing plastic zone as well as the current crack propagation and the *J*-integral in dependence of the crystal orientation and notch geometry.

Keywords: Single-Crystal Tungsten, Microbeam, Fracture Toughness, FE Model, Crystal Plasticity, Cohesive Zone Model

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1. Introduction

Tungsten has been used as a functional material in the lightening industry. Due to its distinct properties it shall be applied as a structural material in future energy applications. Its main advantages are the very high melting point, the high Young's modulus, the high density and the good thermal conductivity. Improvement of the fracture toughness represents one of the challenges due to the brittle-to-ductile transition of tungsten above room temperature.

Rupp et al. (2010) as well as Gludovatz et al. (2010) found a strong influence of the microstructure on the fracture morphology and toughness as well as on the brittle-to-ductile transition temperature in polycrystalline tungsten. The same holds for tungsten single crystals; Riedle (1996) and Gumbsch (2003) found that the fracture toughness of tungsten single crystals varies from 6.2 to 20.2 MPa $m^{0.5}$ by changing the crystal orientation. Until now, investigations have mainly been carried out on the macro-scale. Fracture studies using micro-specimens are very rare with few exceptions such as Wurster et al. (2010 and 2012).

To deepen the insight into the fracture mechanisms in tungsten, an experimental programme has been setup where single-crystalline notched micro-cantilevers are bent with a nanoindenter, performed by Schmitt et al. (2013). Typical dimensions for the free-standing cantilevers are 30 µm and 150 µm in width and length, respectively. In this paper a finite element crack growth model is presented which is based on the cohesive zone method with crystal plasticity as constitutive law. This model allows studying the interplay between cracking and plastic deformation in dependence of crystal orientation and notch geometry.

2. Experimental and Simulation Approach

2.1. Micro-cantilever bending

To determine the fracture toughness free-standing single crystal micro-cantilevers are used. At the scale the experiments are conducted, the sample geometry (e.g. the crack ratio a/W) is limited by the manufacturing process and, thus, the requirements of the ASTM standards (ASTM E399 and E1820) cannot be completely fulfilled. In relation to the cantilever dimensions the plastic zone is very large. The geometry, which was developed, is somewhat related to the specifications of the ASTM standard and allows the preparation of different notch shapes. As schematically shown in Figure 1, the width W of the cantilever is 40 µm, the thickness B_0 22 µm, the length H approximately 150 µm. The crack length a is typically 10 µm.

In the present paper, two different notch types are analyzed: a V notch and a Chevron notch. In the latter case, stable crack growth is expected after crack initiation.

To manufacture several free-standing micro-cantilevers in a row, tungsten single crystals of 3x3x5 mm^3 size were aligned in a specific crystal orientation. The basic sample geometries are carved by a micro electrical discharge machining (µ-EDM) process. The notch is then prepared with a focused ion beam (FIB) perpendicular to the surface. Finally, the gage section is milled with the FIB to a smooth surface finish as shown in Figure 2. Due to the manufacturing process the final geometry differs from the original design dimensions and is inspected by scanning electron microscopy (SEM) prior to testing. More details about the preparation steps are given by Schmitt et al. (2013). In the present experimental study, the specimens are orientated in such a way that fracture occurs in the $\{110\}<1\bar{1}0>$ crack system.

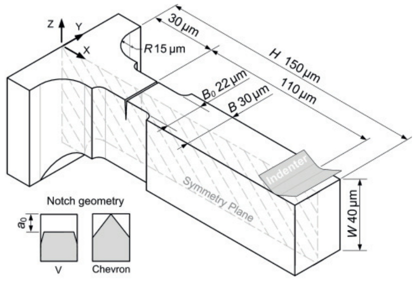

Fig. 1. Specimen geometry of the micro cantilever based on single edge notch bending mimicking crack opening mode I with different notch geometries.

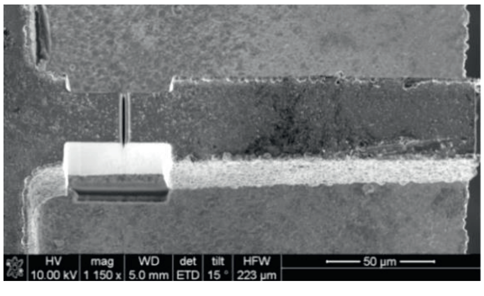

Fig. 2. The Scanning Electron Microscope (SEM) micrograph shows a typical cantilever with cleaned gage section and V-notch which is cut perpendicular to the surface using a FIB.