Journal of Materials Processing Technology 211 (2011) 1305–1323

Contents lists available at ScienceDirect

Journal of Materials Processing Technology

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

Experimental and numerical investigations of the plane strain compression of an oligocrystalline pure copper specimen

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ARTICLE INFO

Article history:
Received 19 January 2011
Accepted 2 March 2011
Available online 10 March 2011

PACS:
81.40.Lm
81.20.Hy
07.05.Tp
02.70.Dh
68.37.Hk
62.20.Fq

Keywords:
Microstructure
Plane strain compression (PSC) test
Oligocrystal
Crystal plasticity
Finite element analysis
Electron backscattering diffraction (EBSD)

ABSTRACT

To evaluate if the deformation in the bulk of an oligocrystalline sample during a plane strain compression test can be accurately simulated numerically with the aid of a crystal plasticity model a detailed comparison between the experimentally found and numerically predicted deformation is made. In the experiment an incremental plane strain compression (PSC) test is conducted on an oligocrystalline specimen. The incremental PSC test is complemented by electron backscatter diffraction (EBSD) measurements. The experimental results enable qualitative observation of the specimen's microstructure and orientation distribution at intermediate stages of the plastic deformation. This incremental PSC test is numerically simulated with the aid of a crystal plasticity finite element model. The numerical model accounts for the specimen's microstructure and the orientations of the crystals. Mapping the microstructure and the grain orientations on the workpiece in the finite element model provides realistic boundary conditions. Both, the experiment and numerical simulation show that the deformation in the oligocrystalline specimen with only a few grains in the deformation zone considerably differs from that of well known continuum like materials. Qualitative comparisons of the incremental PSC test and its numerical simulation showed that most of the experimentally observed behaviour of the grains and their mutual interaction can be seen in the results of the CPFEM simulation as well. From quantitative comparisons it is concluded that the two-dimensional CPFEM simulation can predict the rotations of grains in the bulk of the three-dimensional microstructure of the oligocrystalline specimen only in a qualitative manner. The lack of quantitative agreement is most probably caused by the fact that this two-dimensional, plane strain CPFEM model does not account for the interaction of the grains in the microstructure beyond the analysed cross sectional surface.

1. Introduction

By contrast with common metal forming processes at conventional length scales in the macroscopic domain, the material behaviour of workpieces containing a small number of crystals during metal forming is not like a continuum. Forming such oligocrystals is strongly affected by local deformation, local strain and the effect of local strain rates as well as by phase and grain boundaries, grain size and orientation. Different material phases, a small number of crystals or even a single crystal have a significant influence on the integral behaviour of the grains in the plastic zone. This leads to the fact that simulating a forming process of an oligocrystalline workpiece with the aid of conventional numerical simulation methods based upon continuum mechanics does not meet the accuracy standards. Simulating forming processes of oligocrystalline workpieces requires numerical methods that account for the influence of the microstructure. This can be done in two different ways, either by (slightly) enhancing the well known continuum plasticity models or by applying crystal plasticity models, which directly take the microstructure into account when used with a subgrain resolution of the FE mesh. As the grain structure is the most important of the features mentioned above, this article focuses on accounting for the influences of the individual grains by the application of a crystal plasticity model.

In this article the results of a crystal plasticity model of the deformation up to high strain levels in the bulk of an oligocrystalline pure copper specimen during an incremental plane strain compression test (PSC test), representing a metal forming process, are compared with experimentally obtained results.

This work considers length scales of both the workpiece dimensions and the grain sizes far above several tens of micrometers. On one hand the limited number of grains in the oligocrystalline

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doi:10.1016/j.jmatprotec.2011.03.003

pure copper specimen does not allow a statistical representation of the crystallographic texture. On the other hand the grains are still large enough to neglect the share of the strain gradients at grain boundaries as well as at the free surfaces. The analyses of the experimental results and of the numerical simulation with the crystal plasticity model do not incorporate any material length scale and do not account for size effects due to strain gradient effects. At length scales above several micrometers, conventional plasticity theories which neglect strain gradients usually suffice (Fleck and Hutchinson, 1997). When the length scale becomes smaller, from about a fraction of a micrometer to tens of micrometers, hardening due to the combined presence of geometrically necessary dislocations associated with a plastic strain gradient (generally inversely proportional to the length scale over which the plastic deformation occurs) becomes important. At this length scale, metals and ceramics display strong size dependence where smaller is stronger (Hutchinson, 2000). Metal forming at this very small length scale is not considered in this paper. The grains are large enough to ensure that dislocation slip is the main contributor to plasticity. Effects such as source starvation which are a potential candidate for higher order size effects at length scales from about a fraction of a micrometer to tens of micrometers (Demir et al., 2010), are assumed to be irrelevant at the length scale far above several tens of micrometers considered here.

1.1. Literature review

Simulating the mechanical behaviour of individual crystallites under complex loading is the main strength of the crystal plasticity finite element method (CPFEM) and many applications of CPFEM to calculate the deformation of small sets of crystals can be found in literature. However, only more recent publications show sophisticated comparisons of local data from simulation and experiments. Raabe et al. (2001) and Sachtleber et al. (2002) studied a channel die experiment of a columnar aluminium multi-crystal. As this set-up is quasi two-dimensional the material behaviour can not be assumed representative for the behaviour of grains in a three-dimensional grain structure; moreover the surface friction gives rise to rather ill-defined boundary conditions. Zaefferer et al. (2003) used channel die compression to deform different bi-crystals. Bi-crystals are also not representative for a three-dimensional grain structure. Finally Zhao et al. (2008) studied the tensile test of a polycrystal. However, here the grain structure is again columnar and all grains are surface grains.

While all these works demonstrated the capability of CPFEM to correctly predict the local deformation behaviour of a few (surface) grains, the experimental set-ups chosen are not representative for three dimension microstructures in bulk material.

Quinta da Fonseca et al. (2006) investigated the effect of the grain size on the development of intergranular strains in interstitial free steel by comparing the results of in situ straining neutron diffraction experiments and finite element simulations. The tensile test specimens with a cylindrical cross section of 8 mm in diameter and 80 mm gauge length had mean grain sizes of 80 and 350 μm. The experimentally measured deformations were statistically compared against the predictions of a CPFEM model and matched fairly well. However, the authors did not provide an exact one-to-one comparison of grains in the simulation and the experiment. Kim et al. (2006) experimentally and numerically studied the deformation of pure aluminium specimens composed of a few grains during channel die compression. Polycrystalline aluminium cubes (3^3 mm^3) with grain sizes between 1 and 3 mm were compressed. The surface grain orientations of the initial specimens were measured by EBSD. The specimens were classified into two types: single grain specimens (type 1) and specimens composed of several grains (type 2). The compression of the type 2 specimens was not directly compared with the corresponding FEM predictions; the comparison was made in a qualitative manner by means of the surface profile. The applied crystal plasticity model reasonable described the deformation of the type 2 specimens. The deviations were ascribed to the lack of data of the internal grain structure and orientation distribution. Also in this experiment, the surface grains can not be regarded to be representative for grains in the bulk of a three-dimensional grain structure. Finally it was concluded that a measuring technique for the inner grain distribution is required to predict the actual polycrystalline deformation more accurately. You et al. (2006) performed a detailed comparative experimental and computational analysis of the tensile deformation of a 316LVM stent strut-like specimen. The experimental observations and model predictions were compared on the basis of active slip systems, microscale strain distribution and individual grain reorientations. A portion of the 90×60 μm specimen's gauge length approx. 180 μm long was selected for study. The specimen consisted of only one or two grains across the width. A maximum global strain of approx. 18% was reached in the in situ tensile test. Two different 3D CPFEM model types were constructed: a prismatic model with a through thickness extruded grain structure and a full 3D model with an interpolated grain structure. The results showed that the models gave a good prediction of the global stress–strain curve of the specimen, with the full 3D models being superior to the idealised prismatic grain model. Less successful, however, was the prediction of grain reorientation during deformation and the development of discrete deformation bands within the grains. It was observed, that the reorientation strongly depends on the latent hardening ratio. Musienko et al. (2007) compared an in situ tensile test on a recrystallised OFHC copper specimen with a crystal plasticity simulation of this experiment. The measurements in the experiment focused on a small region of interest on the specimen's surface. After the experiment the three-dimensional structure underneath the area of interest was reconstructed with the aid of an etching procedure. The subsequent numerical simulation considered the volume underneath the area of interest with the reconstructed three-dimensional structure. The initial lattice orientations were taken for the grains lying at the surface and the orientations after the deformation for the grains below the surface. As this volume only represents a small part of the specimen, the five interfacial surfaces had to be constrained by idealised boundary conditions. The comparison was only made for the external surface and not for the bulk. It was concluded that the boundary conditions were absolutely not realistic. Nevertheless, there existed a good general agreement between the computation and the experiment. It is assumed, this is due to the small deformation with a maximum global true strain of 0.095. Musienko et al. proposed that it might be interesting to develop new (statistical) approaches to obtain the bulk's microstructure as well as suitable boundary conditions and experimental data of the bulk. In Geißdörfer et al. (2008) a tool set-up to enable the in situ observation of a miniaturized can backward extrusion process was introduced for the analysis of local deformation behaviour. The punch and the die had a half cylindrical lay-out which was closed by a sapphire window. Through this window the deformation was captured by a CCD-camera. A special image analysis algorithm calculated the local displacement of the material. CuZn15 specimens with mean grain sizes of 104 and 211 μm were used for the investigations. Analysis of the local deformation showed, that the deformation process was significantly influenced by the local grain constellation in the deformation area. The process has been numerically simulated with an enhanced continuum plasticity model, called mesoscopic model (Geiger et al., 2007), and a synthetic material structure. The inhomogenities in the local displacement as well as the influence of the grain size on the punch force, both observed in