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Orientation-dependent evolution of the dislocation density in grain populations with different crystallographic orientations relative to the tensile axis in a polycrystalline aggregate of stainless steel

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Abstract

Line profile analysis was carried out on neutron diffraction patterns collected by the energy-dispersive method for an in situ tensile-deformed AISI-316 stainless steel specimen. The experiments were carried out at the VULCAN engineering beam line of the spallation neutron source of the Oak Ridge National Laboratory. Both the dislocation densities and the local stresses in grains oriented with different hkl crystal directions along the tensile axis were determined. The work-hardening equation of Taylor was tested for the hkl-dependent phenomenological constant α. The grain-orientation-dependent α values were directly related to the heterogeneity of dislocation distribution in correlation with previous transmission electron microscopy data.
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1. Introduction

Structural materials are polycrystalline aggregates composed of single crystal grains with different crystallographic orientations. The elastic–plastic response during deformation is a key issue in work-hardening and mechanical behavior. Modeling started in the 1930s, when Masing [1] suggested that the polycrystalline aggregates behave like composites of individual single crystals. Though the details and methods today are far more advanced, the concept is still valid. One of the methods is the full-field approach using the finite element (FE) method [2,3]. The polycrystalline aggregate is built up by elastically and plastically anisotropic grains of different shape and size where the elastic–plastic response is calculated numerically by the FE method. In the homogenization models the grains are embedded into a statistically averaged mean-field [4,5]. The latter is by far less numerically intensive than the FE method, but the elasto-plastic anisotropy of the surrounding is eliminated by the averaging procedure. The advantages of the two models are merged into a full-field elasto-viscoplastic approach, where the local mechanical fields acting on a grain are calculated by a fast Fourier transform algorithm [6]. The experimental verification of the model predictions requires a knowledge of work-hardening and intergranular strains on the grain scale. One of the key parameters in work-hardening is the α parameter in Taylor's equation [7]. It bridges the critical shear stress, τ, with the dislocation density, ρ. The value of α can only be determined if the two quantities, τ and ρ, are measured independently. The determination of dislocation densities in single grains of a polycrystalline aggregate [8,9] or even in grains corresponding to different orientations along the direction of the applied stress are a special

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challenge. In the present work we determined the dislocation densities in grains oriented with different hkl crystal directions along the applied uniaxial tensile strain. The hkl-dependent lattice strain and the $h/k/l$-dependent line broadening data provided the hkl-dependent stresses, τ_{hkl}, and dislocation densities, ρ_{hkl}, which were evaluated for the hkl-dependent α_{hkl} values in terms of Taylor's work-hardening equation. The results are discussed in correlation with previous tensile experiments on face-centered cubic (fcc) single crystals [10,11], with previous transmission electron microscopy (TEM) investigations of dislocation patterning in tensile-deformed polycrystalline fcc metals [12–14] and the composite model of the α constant in Taylor's equation [15].

2. Experimental

2.1. Experimental set-up

In situ neutron diffraction experiments were carried out in the VULCAN engineering diffractometer [16,17] at the spallation neutron source of the Oak Ridge National Laboratory (ORNL) in Oak Ridge, Tennessee, USA. The schematic experimental set-up is shown in Fig. 1. A threaded dogbone-shape AISI-316 stainless steel specimen of 6.35 mm diameter and 60 mm gauge length was tensile deformed in the 100 kN in tension MTS (Materials Testing System) multiaxial load frame at a constant strain rate of $\sim 4 \times 10^{-5}\ s^{-1}$. The tensile stress axis of the load frame was mounted at 45° against the neutron beam direction. The diffraction patterns were collected by two $2\theta = \pm 90°$ detectors. The two detectors, B1 and B2, collected diffraction from lattice planes perpendicular and parallel to the loading direction, respectively. The macroscopic engineering strain was followed by an extensometer with a nominal gauge length of 12.7 mm. As indicated in Fig. 1, the tensile direction is parallel to the Q_1 diffraction vector, corresponding to the B1 detector bank. Each hkl reflection measured in the B1 detector-bank pattern corresponds to the well-defined hkl-oriented orientation fibers where the local tensile axis, σ_{loc}, is parallel to the direction of the external tensile stress. The arrowed circles in the figure indicate that perpendicular to the orientation fibers the grains are oriented randomly. The corresponding diffraction patterns are obtained in the B2 detector bank with the Q_2 diffraction vector. The experimental set-up is similar to that of the SMARTS diffractometer at the Neutron Science Center at Los Alamos National Laboratory [18].

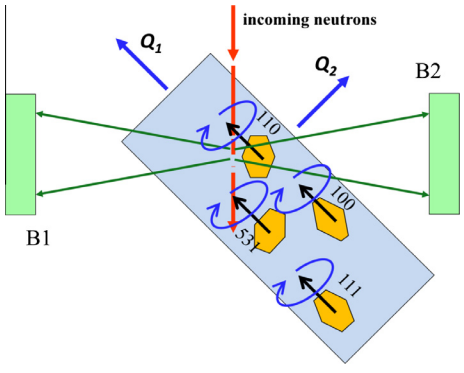

Fig. 1. Schematic experimental set-up with the two detector banks, B1 and B2. Q_1 and Q_2 are the diffraction vectors corresponding to B1 and B2. A few grains are shown schematically with corresponding hkl indices in the Q_1 direction. The arrowed circles indicate that in the Q_2 direction the grain orientations are random.

2.2. The neutron diffractometer

The two detector banks collect the scattered neutrons in sampling volumes defined by the incident beam slits and the radial collimators located between the specimen and the detector banks restricting the field of view to 5 mm along the neutron beam path. Each bank includes three position-sensitive detectors operated as wavelength-shifting fiber scintillator detectors [19]. The horizontal spatial resolution of the detectors is 5 mm, which matches the effective sample size and provides a horizontal angular resolution of 0.2° for a single detector pixel. The total angular coverage of the detectors is $\sim 23° \times 10°$ with 154×7 pixels. The rather large difference in the pixel size along the horizontal and vertical directions is acceptable due to the relative flatness of the diffraction cones for the scattering angles close to ±90°. The diffraction patterns were collected in each detector pixel by using the specific neutron wavelength, λ, which is proportional to the time-of-flight (TOF) interval between the neutron pulse generation and the detection moment. The TOF regime produces the total diffraction pattern in each detector pixel. The different pixel contents are synchronized to the nominal detector-bank center by using the diffraction patterns of a diamond powder sample and creating a look-up table for the shifts in the TOF scales for each single pixel. The diffraction patterns in each single pixel are summarized into one resultant pattern by using the TOF shifts given in the look-up table. We call this procedure time-focusing. At the end the resultant diffraction pattern retains the same good angular resolution as each individual pixel, but the statistics of the pattern becomes greatly improved.

In order to have good reciprocal space resolution in the TOF regime, the sample was located at a long distance of ~42 m from the neutron source. The curved neutron guide [16,17] enables us to get rid of the fast neutrons which are not blocked by the choppers. Since in line-profile analysis the tail parts of profiles are most important [20,21] we used the high intensity mode, with the interchangeable focusing guide system providing 1.6° and 0.2° to 0.6° beam divergence in the vertical and the horizontal planes, respectively [17]. The relatively large bandwidth along with the high TOF resolution was provided by the 30 Hz chopper mode. This corresponds to the bandwidth of wavelength of 2.88 Å centered at 2 Å, corresponding to d values between 0.5 and 2.4 Å, respectively. The angular or d resolution was further improved by radial collimators between the specimen and the detector banks, restricting the field of view to 5 mm along the neutron beam path and the sampling volume to

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