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Effect of local stress heterogeneities on dislocation fields: Examples from transient creep in polycrystalline ice

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Abstract—This work presents a coupled experimental and modeling approach to better understand the role of stress field heterogeneities on deformation behavior in material with a high viscoplastic anisotropy e.g. polycrystalline ice. Full-field elasto-viscoplastic modeling is used to predict the local stress and strain field during transient creep in a polycrystalline ice sample. Modeling input includes the experimental starting microstructure and a validated slip system dependent flow law. EBSD measurements on selected areas are used to estimate the local dislocation field utilizing the Weighted Burgers Vector (WBV) analysis. Areas of local stress concentration correlate with triple junctions and grain boundaries, originating from strain incompatibilities between differently oriented grains. In these areas of highly heterogeneous stress patterns, (a) kink bands are formed and (b) WBV analysis shows a non-negligible *c*-axis component of the WBV. The correlation between this defect structure and presence of kink bands suggests that kink band formation is an efficient accommodation deformation mode.

Keywords: Stress heterogeneities; Dislocation field; Electron backscatter diffraction; Full-field modeling; Kink bands

1. Introduction

When polycrystalline material is plastically deforming, stress and strain heterogeneity fields are developing due to strain incompatibilities between grains of different crystallographic orientations. Depending on the level of viscoplastic anisotropy of the material, the heterogeneity amplitude can be high.

The viscoplastic anisotropy of ice is known to be very strong, with dislocations gliding mostly on the basal plane with three equivalent $\langle 11\bar{2}0\rangle$ Burgers vector directions [1]. This results in strong kinematic hardening at grain boundaries and triple junctions [2]. As such ice is a good model for materials with high viscoplastic anisotropy, such as magnesium [3,4], quartz [5] and olivine [6]. In ice, strong heterogeneity fields were measured by Digital Image Correlation on polycrystalline samples deformed by compression creep with local strain amplitude as high as ten times the macroscopic strain [7]. The strain heterogeneities were also indirectly observed through lattice misorientation measurements via EBSD [8,9] and were simulated using full-field viscoplastic approaches based on Fast Fourier Transform formulation [10,9,7]. In these modeling approaches, plasticity is simulated by the activation of several slip systems (e.g. basal, prismatic and pyramidal slip in the case of ice), where each slip system is assigned a relative critical resolved shear stress for slip activation. In this frame, these last works have shown, among other results, that observed high stress and strain heterogeneities could only be correctly simulated providing a significant amount of non-basal slip activity in the corresponding areas, while the global non-basal activity remained low [10,9]. The same numerical constraint was derived for polycrystalline Mg in conditions where twinning was not activated ([11]). However, up to now there exists no unequivocal evidence for macroscopic strain resulting from non-basal slip in ice [12,13].

The presence of heterogeneous dislocation fields in experimentally and naturally deformed ice was mostly observed indirectly from substructure observations (X-ray diffraction, optical analyzes, EBSD…) [8,9,14,15]. In particular kink bands and double kink bands have been

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commonly observed in polycrystalline ice deformed in the laboratory. The origin of these kink bands was indirectly interpreted to be related to some non-basal dislocation activity like climb or cross-slip [8,9].

The objective of the present work is to couple both modeling and high resolution EBSD observations in order to extract a more direct causal relationship between stress and dislocation fields. These relationships are expected to be of particular significance in polycrystalline materials composed of phases exhibiting a strong viscoplastic anisotropy.

2. Experiment and EBSD analyzes

Both modeling and experimental analyzes were performed on the basis of compression creep experiments on samples made of laboratory grown polycrystalline ice with columnar grain shape [9]. Tests were stopped at 1% strain in order to prevent the initiation of recrystallization processes. A constant 0.5 MPa stress was applied at −10 °C, with columns perpendicular to the compression direction (see [7] for details). Grain size of the order of 1 cm enabled high resolution observations in terms of microstructure and crystal orientation variations at grain boundaries, triple junctions and grain interiors. The deformed microstructure is shown in Fig. 1. In all analyzes the same XYZ sample coordinate system is used where Z is out of plane and the Y direction is parallel to the main compression axis.

EBSD analysis was performed on a Philips XL-30-ESEM-FEG at the Department of Geological Sciences at Stockholm University. EBSD patterns were auto-indexed using the CHANNEL 5 software of OI-HKL Technology. Samples analyzed were extracted from the deformed sample. They were uncoated, kept at high vacuum and frozen to the pre-tilted sample holder sledge cooled to temperature of −90 to −100 °C using a cold stage (for more details see [8]). Data were collected by moving the beam across a rectangular area at steps of 15 μm. Noise reduction was performed following [16,17]. Accuracy of EBSD data is within 0.3°–0.4°[18]. Fig. 1 presents selected EBSD maps showing the local variations in orientations.

3. Weighted Burgers Vector analysis

To quantitatively analyze the EBSD point grid data we utilized the Weighted Burgers Vector (WBV) analysis explained in detail in [19]. The WBV is a recently developed new quantity to constrain dislocation densities and dislocation types using EBSD data on two dimensional sections through crystalline materials. The WBV is defined as the sum, over all dislocation types, of [(density of intersections of dislocation lines with a map) × (Burgers vector)] and as such can be calculated from a planar set of orientation measurements such as in an EBSD orientation map. There is no assumption about the orientation gradient in the third dimension. The magnitude of the WBV gives a lower bound of the magnitude of the dislocation density tensor. The direction of the WBV can be used to constrain the types of Burgers vectors of the geometrically necessary dislocations present in the microstructure and their geometric relationship to intra-grain structures, for example subgrain walls. The WBV can then be decomposed in terms of the 3 main lattice vectors [20]. In the case of ice, the two a-axis lattice vectors are further decomposed into the 3 equivalent a-axis lattice vectors. We can calculate the net Burgers vector content of dislocations intersecting a given area of a map by an integration around the edge of this area. This integral WBV method is fast, complements point-by-point WBV calculations and, thanks to this integration, reduces the effect of noise on the analysis. A lower bound of the density of geometrically necessary dislocations can be estimated from this calculation. This estimation is not absolute but can be used for comparison purposes. It should be noted that the net Burgers vector value derived using the integral WBV method is sensitive to the chosen area both in terms of size and location.

WBV analysis data are represented in color coded maps showing the WBV magnitude, WBV directions as projected arrows onto the color coded maps and in pole figures with both the sample coordinate system and the crystal coordinate system (see Fig. 2).

Table 1 presents the integral WBV calculated over selected areas in the analyzed samples (Figs. 2 and 3), decomposed into the three a-axes and the c-axis of the ice crystallographic structure. Areas were selected to represent the observed spectrum of different microstructures present within the analyzed sample. Such microstructures include triple junctions, grain boundaries with or without asperities, areas in close vicinity or at distance to grain boundaries. Data from Table 1 show that the integral WBV values vary significantly depending on microstructure type and location. However, for each selected area, we obtained several WBV values and chose to present here values that are representative for the selected area.

The accuracy of the integral WBV is dependent on the angular resolution of the EBSD data. Using EBSD data with high angular resolution (here within 0.3 degrees), we consider an integral WBV ratio of one specific Burger vector over the maximum WBV value of 0.5 significant.

4. Local stress field estimation

Full-field numerical simulations were performed using the CraFT code as presented in [21]. The code is based on the FFT method initially proposed in [22,23], extended to elasto-viscoplastic composites using a step-by-step integration in time in [24] (see also the numerical details in [21]). The method used in the CraFT code finds a strain rate field associated with a kinematically admissible velocity field that minimizes the average local work rate under the compatibility and equilibrium constraints. An iterative scheme is used following a fixed point approach. It is numerically more efficient than the finite element method [25], but is limited to simulations with microstructures with periodic boundary conditions.

The specimen undeformed microstructure was discretized into 512 × 512 Fourier points with a single layer of Fourier points in the third (Z) direction, assuming thus infinite column length. To represent the microstructure, each Fourier point is allocated a c-axis orientation according to the measured orientation of the undeformed experimental sample. Consequently grain boundaries are not specifically defined as discrete objects with specific physical characteristics other than a change in crystal orientation. Throughout the numerical simulations, no crystallographic