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# Strain localization in ductile rocks: A comparison of natural and simulated pinch-and-swell structures

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ABSTRACT

We study pinch-and-swell structures in order to uncover the onset of strain localization and the change of deformation mechanisms in layered ductile rocks. To this end, boudinaged monomineralic veins embedded in an ultramylonitic matrix are analyzed quantitatively. The swells are built up by relatively undeformed original calcite grains, showing twinning and minor subgrain rotation recrystallization (SGR). Combined with progressive formation of high-angle misorientations between grains, indicative of SGR, severe grain size reduction defines the transition to the pinches. Accordingly, dynamically recrystallized grains have a strong crystallographic preferred orientation (CPO). Toward the necks, further grain size reduction, increasingly random misorientations, nucleation of new grains, and a loss of the CPO occur. We postulate that this microstructure marks the transition from dislocation to diffusion creep induced by strain localization. We confirm that the development of boudins is insensitive to original grain sizes and single-crystal orientations. In order to test these microstructural interpretations, a self-consistent numerical grain size evolution is implemented, based on thermo-mechanical principles, end-member flow laws and microphysical processes. Applying constant velocity and isothermal boundary conditions to a 3-layer finite element pure shear box, pinch-and-swell structures emerge out of the homogeneous layer through grain size softening at a critical state. Viscosity weakening due to elevated strain rates and dissipated heat from grain size reduction promotes strain rate weakening until a critical grain size is reached. At this point, a switch from dislocation to diffusion creep occurs. This state locks in at local steady states and is microstructurally expressed in pinches and swells, respectively. Thus, boudinage is identified as an energy attractor, identifying the high-energy steady state of an extending layered structure. We conclude from the similarity between natural observations and numerical results that critical deformation conditions of ductile creep can be derived for the surrounding highly-strained host rock matrix.

## 1. Introduction

Boudinage and folding structures are frequently investigated in order to assess the rheology of a creeping material, its mechanical properties as well as the structural evolution. These localization patterns are classically approached either by the study of natural structures (e.g. Goscombe et al., 2004; Hudleston and Treagus, 2010), experimental work or numerical simulations. While classical experimental research has mainly focused on reproducing geometries and describing simplified rheologies (e.g. Abbassi and Mancktelow, 1992; Kidan and Cosgrove, 1996; Neurath and Smith, 1982; Paterson and Weiss, 1968; Ramberg, 1955), numerical simulations have increasingly been used in order to investigate the microphysical framework and the dynamic evolution of the investigated geological structure (e.g. Abe and Urai, 2012; Hobbs et al., 2007, 2008; Mancktelow, 2001; Mancktelow and Abbassi, 1992; Passchier and Druguet, 2002; Regenauer-Lieb et al., 2006; Schmalholz and Fletcher, 2011; Schmalholz and Schmid, 2012; Schmalholz et al., 2008). Direct comparisons between numerical simulations and natural boudinage structures have been the subject of renewed interest (Gardner et al., 2015; Peters et al., 2015; Schmalholz and Maeder, 2012), but a detailed analysis of the mechanics and physics of the phenomenon has not been performed to date. In this contribution, we intend to fill this gap. We present a working hypothesis based on field observations, which is subsequently investigated in depth using numerical methods. We identify and analyze the effects of complex rheological transitions and coupled microphysical relationships postulated in the foregoing analysis of natural microstructures.

The ductile class of boudinage, expressed by symmetric pinch-and-swell structures (*drawn* boudins in the nomenclature of Goscombe et al., 2004), has recently been interpreted as the result of visco-plastic deformation of a power-law layer (Schmalholz and Maeder, 2012; Schmalholz et al., 2008). In contrast, Gardner et al. (2015) have presented a combined *Mohr–Coulomb* strain localizing

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behavior linked with subsequent viscous creep for the initiation of pinch-and-swell structures. In the latter study, the inception of boudinage was controlled by an intrinsically unstable (brittle) material behavior, after which the material was allowed to creep in a ductile manner. In the ductile field, Schmalholz and Maeder (2012) implemented small-scale heterogeneities focussing strain and resulting in localization. The underlying localization criterion was provided by the study of Fletcher (1974), in which a linearized power-law material behavior was considered. The introduced heterogeneities are thought to stem from pre-existing structural perturbations, i.e. geometric interactions caused by structural, material, and inherited rheological imperfections or a combination thereof. The application of such imperfections seems to be an appealing concept for geological applications, as their appearance can be justified from the heterogeneities or inherited structural patterns (anisotropy) of real materials (e.g. Mancktelow and Abbassi, 1992; Paterson and Weiss, 1968; Rybacki et al., 2014). Another advantage from a technical point of view is that small geometric perturbations of a numerical mesh are useful in order to avoid the mesh-sensitivity of numerical simulations, but their seed requires a robust analysis of the localization problem (Peters et al., 2015). The concept of pre-existing weaknesses has, however, recently been challenged by e.g. Hansen et al. (2012), who suggested that localized deformation appears irrespective of the presence of structural heterogeneities under a constant stress boundary condition. For constant strain rate boundary conditions, these authors postulated a critical imperfection size or strength to be met in order to trigger localization.

Localization phenomena can be discussed in further details when explicitly calculating the energy flows during deformation, thus allowing the assessment of complex feedback phenomena. To this end, an energy-based framework of localization has been proposed and applied to simple generic case studies (e.g. Hobbs et al., 2011, 2007, 2009; Regenauer-Lieb et al., 2006; Regenauer-Lieb and Yuen, 2003, 2004). In this energy framework, heterogeneities are a possible seed, but not a necessary condition for localization to appear. On the contrary, the coupling of the temperature-stress evolution to the mechanical properties of the material is of great interest. While a theoretical discussion of this concept is readily available in literature (*ibid*.), a direct application to natural localization structures has not been provided yet. Such a comparison would not only allow an assessment of whether the theory can be further applied than solely investigating the physics of localization. We therefore not only want to use the approach to shed light on the poorly understood driving mechanisms or the creep regime for the initiation of boudinage, but also try to predict a useful application to the field. We therefore strive at uncovering the onset of boudinage in a ductile material by means of a detailed microstructural analysis of natural pinch-and-swell structures and numerical analyses, posing the following questions:

(i) Based on a microstructural study, can we provide insights into the mechanisms driving the onset of boudinage? How do grain sizes, textures and deformation mechanisms progressively adjust during the different stages of deformation?
(ii) Can pinch-and-swell structures be described as a rheological instability? In other words, are geometric-material imperfections essential, or can we find evidence of localization from homogeneous state at the scale of observation?
(iii) What is the physical relationship between microstructure (grain size, texture, deformation mechanism), material properties (thermal-mechanical, grain size reduction and growth parameters), and the deformation conditions (stress, strain rate, temperature)?
(iv) Based on numerical simulations, can the microstructural evolution and the natural creep conditions during boudinage and of the surrounding host rock matrix be quantitatively assessed?

## 2. Microstructural methods and sample description

We studied various undeformed and low-grade boudinaged calcite veins embedded in an ultramylonitic matrix (host rock). Detailed microstructural studies of one representative sample shall be presented in the following. The specimen was cut parallel to the mineral lineation (L) and perpendicular to the foliation ($f_n$), prepared for a thin section of 30 μm thickness, mechanically polished with a diamond paste, and further chemo-mechanically polished with colloidal silica for electron-backscatter diffraction analysis (EBSD). High-resolution imaging and EBSD measurements were performed using a *ZEISS Evo 50* scanning electron microscope, allowing crystal orientation mappings by means of EBSD (*TSL/Ametek* system). The setup was run under low-vacuum conditions (10–15 Pa) at 15 nA beam current and 20 kV acceleration voltage. In order to resolve individual grains, the applied step sizes varied between 0.5 and 10 μm for different study sites. Individual grain boundaries were found by means of the comparison of misorientation angles between neighboring points in the grain orientation map through the distinction between low-angle (<15°) to high-angle grain boundaries (>15°). A standard data clean-up procedure was performed (e.g. Rybacki et al., 2014) by standardization of the confidence index (CI) of different points and subsequent neighbor CI correlation of 0.1, removal of points with an CI< 0.1 and one step of grain dilation, considering a minimum grain tolerance angle of 15° for a minimum grain size of 5 correctly indexed points. Pole figure diagrams of grain orientations, presented as upper hemisphere, equal-area projections, using linear contouring for plots per point, are displayed in the vertical direction of finite strain ($f_n$) and parallel to the mineral lineation (L). We further computed the fabric strength (J) and maximum intensity ($I_{max}$) of the textures. Finally, area-weighted mean recrystallized grain sizes ($\bar{d}_{area}$) were calculated, as the grain size class of the largest grain fraction was found to dominate the bulk rheology of monomineralic aggregates (e.g. Berger et al., 2011; Herwegh, 2000; Shimizu, 2008).

Low-grade sedimentary nappes serve as excellent study areas for the investigation of the natural creep conditions of the uppermost ductile crust (e.g. Austin and Evans, 2007, 2009; Austin et al., 2008; Barnhoorn et al., 2004; Bestmann et al., 2000; Burkhard, 1990; Ebert et al., 2007a, 2007b; Herwegh et al., 2005; Herwegh and Pfiffner, 2005; Renner et al., 2002). In such a setting, monomineralic veins are often formed synkinematically, while they are embedded in a creeping, high-strain matrix of the host rock. This setting allows us to determine creep conditions of these layers varying between the pre- to post-localized states, which can later be potentially upscaled for tectonic processes. For these reasons, we present a detailed microstructural investigation of boudinaged pure calcitic veins, sampled in the Doldenhorn nappe of the Helvetic Alps (Switzerland). The Doldenhorn nappe forms the central part of the nappe stack of the Helvetic Alps, overlying the Gastern granite as part of the external crystalline basement of the Central Swiss Alps (Herwegh and Pfiffner, 2005). For this study area, a rich dataset of the paleo-deformation conditions was assembled that describe the main episode of thrusting. The record comprises calcite–graphite thermometry on organic nano-flakes defining the foliation and calcite grains from ultramylonites (Herwegh and Pfiffner, 2005), estimations of deformation rates through the *Paleowattmeter* scaling relationship (Austin et al., 2008), and geodynamic constraints on Alpine orogeny (Burkhard, 1988; Herwegh et al., 2005). While the emplacement of the nappe potentially lasted ca. 10 Ma (Herwegh et al., 2005), regional anchizonal to lower greenschist metamorphic conditions endured for around 2–5 Ma (Arkai et al., 2002). Herwegh and Pfiffner (2005) characterized the majority of deformation structures as highly localized thrust faults. For the deformed *Quintnerkalk* sample presented here, a minimum deformation temperature of ca. 350 °C was obtained. Microstructures associated with retrograde shearing mostly appear as cataclasites, which significantly differ from those of the main ductile deformation event. Thus, we assume that temperature is isothermal at least at the scale of the hand specimen. Deformation rates, based on