Journal of Structural Geology 76 (2015) 22–34

Contents lists available at ScienceDirect

Journal of Structural Geology

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

A phenomenological numerical approach for investigating grain size evolution in ductiley deforming rocks

Andrew J. Cross [a], [*], Susan Ellis [b], David J. Prior [a]

[a] Department of Geology, 360 Leith Walk, University of Otago, Dunedin 9056, New Zealand
[b] GNS Science, 1 Fairway Dr., Avalon, Lower Hutt 5011, New Zealand

ARTICLE INFO

Article history:
Received 30 October 2014
Received in revised form
29 March 2015
Accepted 3 April 2015
Available online 23 April 2015

Keywords:
Grain size evolution
Ductile deformation
Numerical model
Piezometer
Grain growth
Dynamic recrystallisation

ABSTRACT

The sizes of recrystallised grains in exhumed ductile shear zones are often used to infer conditions of deformation (i.e. stress, strain rate and temperature). Here we present a simple numerical method of calculating the dynamic evolution of grain size during ductile deformation. Our phenomenological method is based on the fact that the dynamic competition between grain growth and recrystallisation will drive grains towards a steady-state size. At each time increment, grain growth and reduction contributions are calculated, with magnitudes which depend on the difference between the current grain size and a desired steady-state grain size. In our models we use a recrystallised grain size piezometer to calculate the steady-state grain size for a given stress. Our numerical routine is incorporated into the SULEC finite element package, allowing us to explore spatial and temporal changes in grain size.

As a test, we compare model results to measured grain sizes in quartz layers thinned and recrystallised around rigid garnet porphyroclasts under simple shear dominated deformation in the Alpine Fault Zone of New Zealand. Numerical models are able to replicate observed grain size variations, with boundary conditions consistent with those constrained for the central Alpine Fault Zone.

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1. Introduction

Below the seismogenic zone, increasing lithostatic pressures suppress brittle processes and increasing temperatures promote continuous distributed deformation in ductile shear zones, rather than on localised fault planes (Ramsay, 1980). Within these zones, deformation occurs either by the generation and motion of dislocations at high stresses, or by the diffusion of material under low stress conditions. In the boundary region between grain size insensitive dislocation creep and grain size sensitive diffusion creep, it is anticipated that a balance between grain growth and reduction mechanisms under steady-state deformation, prevents runaway rheological weakening by dynamic recovery and recrystallisation (De Bresser et al., 1998, 2001). Thus, the grain sizes of exhumed ductile rocks provide information on the magnitude of stress under which deformation occurred, which when combined with a rheological flow law can elucidate temperature and strain rate conditions, provided that limited post-deformational grain growth has occurred.

1.1. Grain size evolution

It is widely accepted that under steady-state conditions, an inverse relationship between recrystallised grain size and differential stress exists (Poirier, 1985). With increasing stress, the number of free dislocations in a material increases (Kohlstedt and Weathers, 1980; De Bresser, 1996) requiring recovery of dislocations by dynamic recovery and recrystallisation associated with grain size reduction. An expression for the relationship between recrystallised grain size, d and differential stress, σ was first derived for geological materials by Twiss (1977), based on the assumption that the ordering of dislocations into subgrain and recrystallised grain boundaries is an energetically favourable process. In the following years, many other 'paleopiezometric' relationships were derived primarily from experimental data on monophase aggregates, and commonly appear in the form:

$$d = A\sigma^{-b} \tag{1}$$

where A and b are empirical material constants.

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[*] Corresponding author. Department of Earth and Planetary Sciences, Washington University in St. Louis, 1 Brookings Drive, St. Louis, Missouri 63130, USA.

E-mail addresses: ajcross89@gmail.com (A.J. Cross), s.ellis@gns.cri.nz (S. Ellis), david.prior@otago.ac.nz (D.J. Prior).

http://dx.doi.org/10.1016/j.jsg.2015.04.001
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The field boundary hypothesis of De Bresser et al. (2001) explains the development of a steady-state grain size by stating that under stable physical conditions, grains will evolve towards the boundary between grain size sensitive (GSS) and grain size insensitive (GSI) creep, where the ratio of strain rate contributions from dislocation and diffusion creep is unity.

Curiously, many laboratory-calibrated piezometers do not directly overlie the field boundary, yet lie sub-parallel to it (see Fig. 1 in Austin and Evans, 2009). Since the flow behaviour and recrystallisation of a crystalline material are both determined by dislocation dynamics and strain energy, both the flow law and piezometer should be strain rate and temperature dependent. However, in a series of deformation experiments on quartz, Stipp et al. (2006) found no water content, temperature or strain rate dependence of recrystallised grain sizes. Maybe this reflects the fact that only a relatively narrow range of conditions can be explored by laboratory experiments, although the paleowattmeter of Austin and Evans (2007, 2009), which is a stress, strain rate and temperature dependent alternative to grain size paleopiezometry, also predicts the discrepancy between the field boundary and steady-state grain size.

Further complications arise from the fact that while the De Bresser et al. (2001) model of grain size evolution is valid for monophase aggregates, in nature multiple mineral phases are often present together. In such a case, grain size evolution is restricted by the inhibition of grain boundary migration through a process called Zener pinning (Smith, 1948; Evans et al., 2001). Grain boundary pinning limits or entirely prevents the coarsening of grains, perturbing the dynamic balance of grain growth and recrystallisation, and leading to an unimpeded reduction in grain size and a transition to grain size sensitive deformation, so long as dislocations continue to be generated (Bercovici and Ricard, 2005; Warren and Hirth, 2006; Mehl and Hirth, 2008; Herwegh et al., 2011; Linckens et al., 2011). Grain boundary pinning has been proposed as essential to the development of plate tectonics, by enabling shear localisation to form plate boundaries in the early Earth (Bercovici and Ricard, 2013 and references therein).

1.2. Previous approaches to modelling grain size evolution

The idea of modelling grain size evolution in ductile shear zones is not a new one. Most previous approaches are based around the assumption that over time, a microstructure will evolve towards a steady state relationship between stress and grain size. While the evolution towards microstructural steady state is explained by the field boundary hypothesis of De Bresser et al. (2001), the numerical approaches applied in previous studies are quite varied and are summarised here.

Montési and Hirth (2003) approached the problem of modelling grain size evolution by modifying the field boundary hypothesis to address the discrepancy between the theoretical steady-state grain size-stress relationship of De Bresser et al. (2001) and empirically derived paleopiezometers (see Fig. 1 in Austin and Evans, 2007, 2009). In their study, Montési and Hirth allowed grain size to evolve towards a paleopiezometer (defined as in Eq. (1)), rather than the field boundary line. For grain sizes smaller than the stable grain size, the authors calculated grain size evolution using the standard grain growth equation (see Eq. (4) below), and for grain

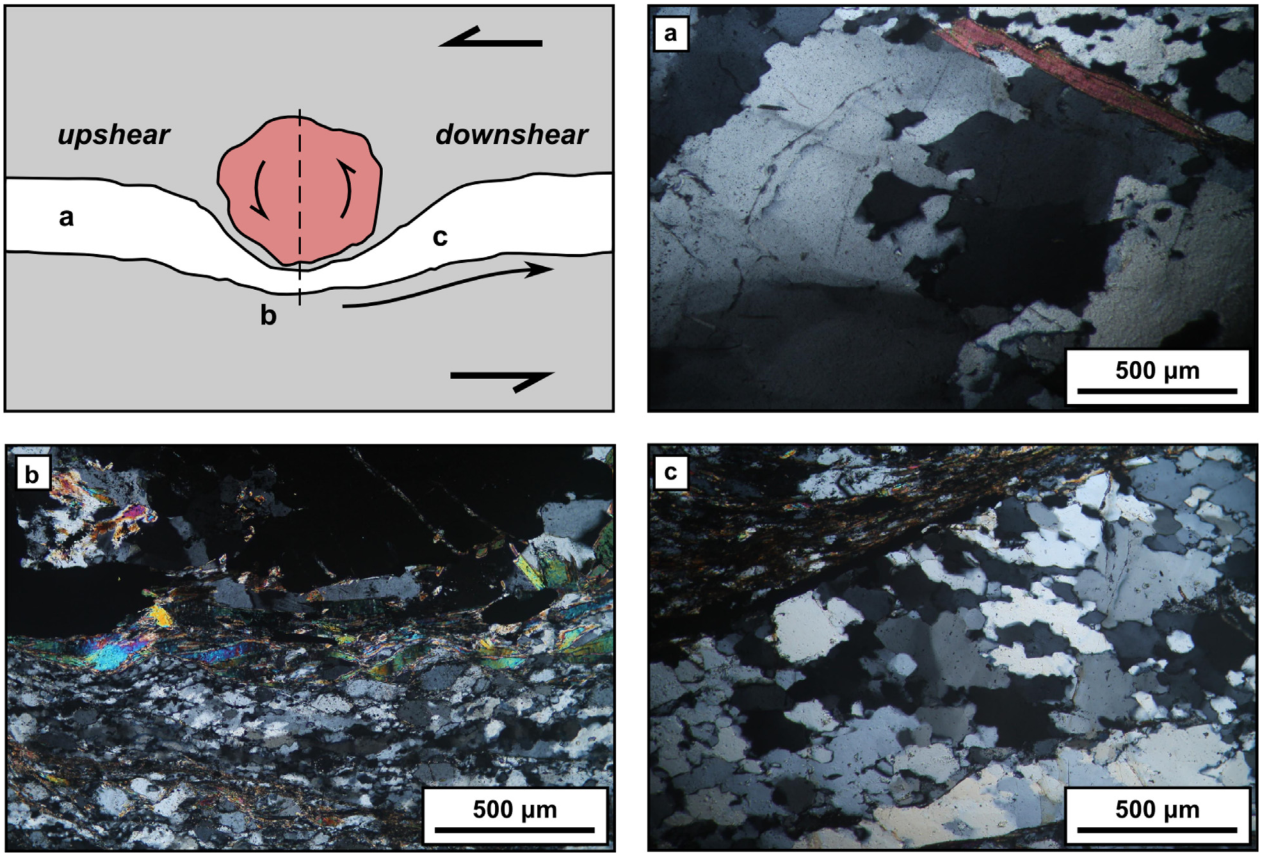

Fig. 1. Typical quartz microstructures along a deflected quartz layer. (a) Upshear of a garnet porphyroclast, quartz grains are large and internally distorted, with lobate boundaries indicative of rapid grain boundary migration. (b) Adjacent to the porphyroclast, grain sizes are significantly reduced. (c) Grains grow downshear of the porphyroclast, with polygonal shapes and little internal distortion.

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