Microphysics of viscoplasticity in Earth's interior

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Motivation

The rheological behavior of the solid Earth fundamentally controls a wide variety of geodynamic processes. The elastic and anelastic behavior of rocks controls the velocities and attenuation of teleseismic waves (Cooper, 2002; e.g., Faul and Jackson, 2015); the linear and nonlinear viscoelastic behavior of rocks controls the vertical motion of Earth's surface in response to changing ice loads (e.g., Ivins et al., 2013), the transfer of stresses on seismogenic faults after large earthquakes (e.g., Freed, 2005), and the response of planetary and exoplanetary bodies to tidal stresses (Ferraz-Mello et al., 2008; Nimmo and Faul, 2013; Zanazzi and Triaud, 2019); the plastic behavior of rocks controls the flexure of the lithosphere near volcanic loads (e.g., Zhong and Watts, 2013) or at subduction zones (e.g., Hunter and Watts, 2016); and the viscous behavior of rocks controls the formation and longevity of plate boundaries (e.g., Bercovici, 2003), the coupling of plates to the convecting interior (e.g., Tackley, 2000), and the styles of convection in the asthenosphere.

Each of these applications interprets geophysical observations with the aid of calibrations of material properties and behaviors from the laboratory. However, extrapolation is always necessary to apply laboratory results to geological phenomena, whether it be in timescale, lengthscale, stress, temperature, grain size, etc. Robust extrapolations can only be made with the aid of constitutive models based on the microphysics of the process in question. Therefore, testing and revising microphysical models for the rheological behavior of rocks is of paramount importance in the study of solid-Earth processes.

An example of the need for detailed understanding of the microphysics of rock deformation is given in Figure 1. Models for dislocation creep of olivine have been used extensively for predicting the viscosity of the upper mantle. These models are fundamentally based on the notion that dislocation climb velocities control the overall deformation rate (e.g., Kohlstedt, 2006). In contrast, recent models based on the balance between dislocation climb and the increase in internal stress heterogeneity result in much more complicated behavior (Hansen et al., 2021; Breithaupt et al., in review) and predict potentially vastly different viscosities when extrapolated to the low stresses and strain rates characteristic of Earth's interior.

Here we outline several example subtopics in the rheology of rocks that all require further investigation of the inherent microphysics to make confident predictions at geological conditions. The common theme is in testing microphysical models of deformation, and we

emphasize that useful tests of these hypotheses are often achieved by going to extreme conditions, even if those conditions are not specific analogs for conditions in Earth. In most cases, the extreme conditions necessary to test these hypotheses are only available at synchrotron facilities, and we discuss how beamline science allows these subtopics to be addressed. Furthermore, we outline future technological advances that would open even more opportunities at beamline facilities for testing outstanding and critical hypotheses.

Outstanding questions, current barriers, beamline solutions, and needs for innovation

Plasticity and strain hardening

Outstanding questions: Plastic yield and subsequent strain hardening of minerals and rocks is a fundamental aspect of rheological behavior at low temperatures, with applications to flexure of the lithosphere (e.g., Zhong and Watts, 2013) and friction on faults (e.g., Aharonov and Scholz, 2018), among others. Yield strength has been investigated in several mineral systems, although results between different studies are often disparate. Some of this disparity arises from differences in microstructural aspects of the samples or in differences in experimental techniques (Kumamoto et al., 2017). Many of these factors have been characterized in olivine to build constitutive models describing yield and strain hardening as functions of microstructural state variables like grain size and dislocation density (e.g., Hansen et al., 2019). Several key questions remain:

- Can models of yield strength and strain hardening based on the grain size and dislocation density be extended to other key mineral systems (e.g., quartz, feldspar, pyroxene)?
- Can existing constitutive models be extended to include the role of other defects (twinning, lamella formation, kinking)?
- How does the addition of secondary phases modify yield and hardening?
- What is the role of volatiles in plasticity of minerals?
- Can these models of plastic deformation be incorporated into descriptions of the brittle-ductile transition?

Current barriers:

Temperature - The primary difficulty in investigating the plasticity of geological materials is their relatively high yield strength at low temperatures. To prevent brittle deformation and isolate plastic deformation, confining pressures must be high (e.g., >6 GPa) at room temperature. Indentation techniques can achieve these conditions, but interpretation of those data is exceedingly difficult. High pressure apparatus are available that can achieve these conditions, but external measurement of the sample state is noisy and biased by the apparatus mechanics. High

temperatures can be applied to reduce the yield strength, but temperature measurement is often not precise enough and additional deformation mechanisms begin to operate, complicating interpretation (Dixon and Durham, 2018). Finally, determination of yield stresses from traditional mechanical testing procedures are often subjective.

Sample Size - Another challenge for current high pressure experiments is the very small sample size (1 to 2 mm) permitted in sample assemblies required to reach pressures relevant to Earth's mantle. It is not clear that such small samples contain the representative volume of material necessary to measure deformation processes dominant in grain interiors, rather processes dominant on grain boundaries. This scale issue may account for some inconsistencies in existing data sets.

Beamline solutions: The original impetus to develop synchrotron based rock deformation experiments was to take advantage of X-ray diffraction to measure the stress within the sample (e.g., Wang et al., 2003). Radiography to measure sample strain and simultaneous X-ray diffraction to measure sample stress circumvent many of the issues mentioned above for high-pressure apparatus. Machine effects are removed when stress and strain of the sample are measured directly, rather than remotely via the use of load cells and displacement transducers. Although stresses measured by X-ray diffraction are complicated by plastic anisotropy of the material (e.g., Dixon and Durham, 2018), the large stresses inherent to plastic deformation at low temperatures provide excellent signal to noise. Furthermore, X-ray diffraction data provides a rich stream of information about plastic deformation mechanisms operating in the sample (e.g. Li et al 2004; Burnley and Zhang, 2008; Burnley and Kaboli, 2019) as well as the development of fabric within the sample(e.g., Bollinger et al., 2012). In situations for which interpretation of diffraction data from the sample is not feasible, either because the diffraction patterns are too complex or incomplete due to large grain sizes, recent efforts have established that isotropic materials can be used as load cells within solid-media apparatus, greatly improving stress resolution (Girard et al., 2020). Radiography of experiments with multiple samples deformed in series also allows the yield point of the weaker experiment to be determined precisely (e.g., Hansen et al., 2019).

Scope for future innovation: As noted above, a key source of uncertainty in existing beamline techniques involving high-pressure deformation is temperature measurement. Common sample assemblies and furnace designs result in considerable temperature gradients across samples. Furthermore, thermocouples in sample assemblies lead to mechanical instability of the assembly, so many experiments are conducted without thermocouples and no direct temperature measurement, leading to significant temperature uncertainties. *Therefore, any improvement allowing more reliable and precise temperature measurement will greatly expand the range of hypotheses that can be tested with these techniques*. There is potential for this difficulty to be overcome by more intimate combination of modeling and experiment, considering that the lattice strain measured by X-ray diffraction also contains information about thermal expansion.

Internal stress distributions

Outstanding questions: The stress state within deforming materials can be heterogeneous due to the inherent heterogeneity of the material microstructure. Internal stresses can build up locally as grains slide past each other on grain boundaries and interact at triple junctions (Crossman and Ashby, 1975; Raj and Ashby, 1971) or as grains of a specific orientation yield while others only deform elastically (Crossman and Ashby, 1975; Duval et al., 1983). Internal stresses can also build up as lattice dislocations interact and generate long-range stress fields (e.g., Bayley et al., 2006). Recent work using *ex situ* electron diffraction has demonstrated that residual stress heterogeneity in ductilely deformed rocks can be surprisingly large, and even an order of magnitude larger than the applied stress (Wallis et al., 2020, 2019). The evolution of internal stress heterogeneity at small scales appears linked to transient creep that likely characterizes postseismic deformation at large scales (Wallis et al., 2021). Internal stresses can also lead to anelastic strain when a material is unloaded (e.g., Faul and Jackson, 2015; Gribb and Cooper, 1998), and therefore are intimately tied to seismic attenuation, postseismic creep, and glacial isostatic adjustment. Several key questions remain:

- Are recent *ex situ*, 2-D estimates of stress heterogeneity accurate characterizations of *in situ*, 3-D stress states?
- What microstructural features (e.g., dislocations, subgrain boundaries, grain boundaries) control the internal stress heterogeneity?
- How does the internal stress heterogeneity scale with the applied stress, temperature, grain size, or dominant deformation mechanism?
- What mechanisms counteract the build up of internal stresses (e.g., dislocation recovery, grain-boundary migration)?
- How do secondary phases affect the internal stress distribution?

Current barriers: Most investigations of internal stress heterogeneity in rocks have either been conducted *ex situ* or by indirect means. *Ex situ* investigation by electron diffraction (Wallis et al., 2019) is relatively new for geological materials and exhibits great potential. However, there is a possibility for stresses to relax during unloading at the end of the experiment. In addition, the sectioning of the sample to prepare a surface for analysis relaxes all stresses normal to the plane and some in-plane stresses (Britton and Wilkinson, 2012). Indirect methods involve measuring the macroscopic anelastic response of a sample to get the net internal stress (Argon and Takeuchi, 1981; Blum and Finkel, 1982; Gibeling and Nix, 1981), but these methods do not resolve the heterogeneity or how it relates to the microstructure.

Beamline solutions: X-ray diffraction techniques have been extensively used for mapping stress heterogeneity in crystalline materials. Adaptation of these techniques to synchrotron X-ray sources has allowed unprecedented improvements in spatial resolution and even 3-D mapping of

stress distributions within samples away from surfaces. These techniques include high-energy diffraction microscopy (Cherukara et al., 2018; Poulsen, 2012), diffraction contrast tomography (Ludwig et al., 2008), and Laue microdiffraction (Hofmann et al., 2010; Robach et al., 2014). Initial results of application of these techniques to naturally deformed rocks are encouraging (Chen et al., 2015), and a clear next step is to use similar techniques on rocks previously deformed in the laboratory under known conditions. Application of microdiffraction to experimentally deformed rocks will allow the internal stress heterogeneity to be quantitatively related to the macroscopic conditions of deformation.

Scope for future innovation: Existing beamline facilities are in place for *ex situ* analysis of deformed rocks using X-ray microdiffraction. However, facilities are not currently available for *in situ* microdiffraction under conditions producing viscous deformation of rocks characteristic of processes in Earth's deeper interior. *In-situ* microdiffraction has been performed on deforming metals (e.g., Collins et al., 2015), but the existing apparatus cannot reach high enough pressures and/or temperatures to suppress fracture in brittle geological materials. A key target for future development is design of beamline facilities to allow microdiffraction in apparatus that generate high pressures and/or temperatures, although the X-ray energies employed will likely need to be increased relative to those typically used for microdiffraction if samples are to be investigated within sealed pressure vessels.

An alternative characterization technique is high-energy diffraction microscopy (HEDM), which provides spatially located information about grain orientation and stress state. However, there is a trade off for this technique between spatial resolution (best in near-field HEDM) and stress resolution (best in far-field HEMD), making it difficult to measure stress heterogeneity within individual grains. Current developments in this technique are moving towards making stress measurements available with higher spatial resolutions (e.g., Shen et al., 2020).

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