Plastic Deformation in Olivine Polycrystals:In-situ diffraction and EPSC models

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Introduction

An important problem in rock deformation studies is the so-called meso-scale problem; understanding how the behaviour of individual mineral grains deforming via grain-scale processes interact to produce the bulk behaviour of the aggregate. A number of models for thinking about this problem exist, ranging from various averages of isolated grain behaviour to those that are dominated by grain configuration, for example stress percolation (as observed in granular materials). It is likely that the degree to which any given model is useful for a particular material depends on the degree of mechanical heterogeneity and anisotropy of the material. We are investigating the deformation of polycrystalline olivine in this light.

Methods

We report on in-situ synchrotron x-ray diffraction from high pressure deformation experiments conducted using olivine in the D-DIA apparatus at beamline X17b2 at the NSLS. We observe the diffraction behaviour of x-ray reflections for lattice planes oriented nearly perpendicular to compression and at several other orientations including the transverse orientation. Sample strain is measured using radiograph of the sample (which is bounded by metal foils). We used elastic plastic self-consistent (EPSC) modelling[1] to analyse diffract-tion from the sample during deformation. The models assume that rheology of the bulk is controlled by the critical resolved shear stress of the slip systems and the orientation of the grains in the polycrystal.

Results and Discussion

The failure of the known olivine slip systems to meet the von Mesis criteria for arbitrary shape change causes the EPSC models to exhibit very strong work hardening and nearly elastic behaviour for many grain populations. This is in stark contrast to our experimental data which consistently shows little or no work hardening after yield.

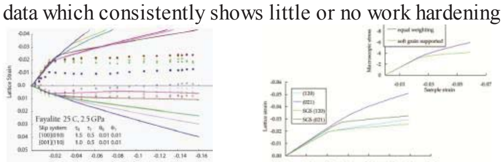

Figure 1: a) (left) Experimental diffraction results (points) for the (021), (010), (120), (002), (131) and (112) lattice planes in compression (above axis) and transverse directions (below axis). EPSC model is shown with matching coloured lines. **b)** (right) Modified EPSC model in which weakest grains dominate.

One possible reason that the deformation behaviour of polycrystalline olivine cannot be predicted with the EPSC model is that grains in the polycrystal that are well oriented for slip (soft grains) dominate the deformation behaviour or the aggregate, with grains that are not well oriented for slip passively "riding along" and not contributing to the aggregate strength. To test this, we assign a weighting factor to each grain depending on the degree of plastic strain that accumulates in the grain during deformation. Using this strategy the EPSC model more closely mimics the lack of work hardening as well as smaller difference in lattice strain between the (120) and (021) reflections.

[1] Turner and Tome (1994) *Acta Metallurgica Materialia* **42**(12) 4143-4153

Integrated 3D multimodal CARS microscopy, Raman spectroscopy, and microthermometry of gas-rich inclusions in the Marcellus shale-gas system

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Gas-rich inclusions in fracture filling cements in the Marcellus Shale and younger Devonian age formations in the Appalachian basin record a complex history of gas generation, migration, and alteration during evolution of the Alleghenian orogen[1]. Quartz and calcite cements contain multiple overlapping fluid inclusion assemblages (FIAs) formed during crystal growth and deformation. To resolve the complex sequences of gas generation and migration recorded by FIAs we applied a nonlinear optical microscopy method capable of 3D, molecule-specific imaging with sub-micrometer resolution: multimodal coherent anti-Stokes Raman scattering (CARS) microscopy. Our implementation of CARS microscopy[2] produces molecule-specific images in the range of 2100 to 4000 cm^{-1} (N_2, CH_4, H_2O) and simultaneously creates second harmonic generation (SHG) images of inclusions with associated quartz microstructures, and two-photon excitation fluorescence (TPEF) images of higher hydrocarbons. The CARS images show the distribution of methane-rich and aqueous phases in inclusions and the TPEF images show the distribution of gas-rich inclusions that contain trace levels of higher hydrocarbons. Individual gas-rich inclusions within distinct 3D FIAs identified with multimodal CARS were analyzed by conventional confocal Raman spectroscopy for minor components (C_2H_6, CO_2, H_2S, N_2) and internal pressure[3]. 2D maps of inclusions with microthermometric measurements were correlated with 2D projections of 3D SHG images. Integration of measurements on individual inclusions with 3D images allows identification of FIAs with distinct spatial orientation and differences in composition (C_2H_6, CO_2, higher hydrocarbons) and density. 3D imaging with CARS microscopy is a major advance in our ability to assign FIAs with distinct compositions to distinct orientations of microstructures formed during kinematic evolution of the orogen. These observations provide new insight to the temporal evolution of hydrocarbon gas generation and migration during evolution of the Marcellus shale-gas system.

[1] Evans (2010) *Geol. Soc. Am. Mem.* 206. [2] Pegoraro *et al.* (2010) *App. Phys.* 49, F10–F17. [3] Lu *et al.* (2007) *GCA* 71, 3969–3978.