Preferred Orientation in ε-Fe under High Pressure and High Temperature

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Introduction

Seismic and free oscillation observations suggest that the solid inner core of the Earth may be anisotropic. This has been interpreted as a manifestation of intrinsic elastic anisotropy, preferred orientation, and texture of the major constituent of the inner core, ε-Fe. Preferred orientation can originate from growth, flow-induced Maxwell stresses, or thermal convection. In conjunction with the elastic anisotropy of ε-Fe, the alignment of the crystals could explain the observed seismic anisotropy.[1] Therefore, the understanding of the elastic and rheological properties of ε-Fe under high pressure and high temperature is of considerable interest.

Deformed polycrystals frequently show a nonrandom orientation distribution. Conventionally, x-ray or neutron diffraction has been used to determine orientation distributions, but most of these experiments are done at ambient pressure, and there is a growing interest in the study of high-pressure phases that are not stable at atmospheric pressure and must be studied *in situ*. We present here new developments to study the evolution of texture in a sample under high pressure and high temperature. Documenting the evolution of texture at high pressure will allow determination of deformation mechanisms (i.e., slip systems) and elastic properties of the appropriate polycrystals.

Materials and Methods

All experiments were performed at the GSECARS Sector 13 of the Advanced Photon Source (APS) at Argonne National Laboratory. Very fine grained iron powder (grain size < 1 µm) was loaded into a diamond anvil cell. To enhance the effect of nonhydrostatic stress and allow laser heating of the sample, we used MgO as a pressure medium. Using x-ray transparent gaskets made made of amorphous boron and epoxy, we performed angular dispersive diffraction with the incoming x-ray beam perpendicular to the load axis (Fig. 1). Patterns were collected on an imaging plate, and we studied the variation of the diffraction angle 2θ and intensity as a function of the azimuth angle on the imaging plate δ.

The sample was heated using a double-sided Nd:YLF laser heating system, as described in Ref. [2]. Equivalent hydrostatic pressures were determined using the equation on state of ε-Fe itself.[3] Thermal radiation was collected from both sides of the sample surface and dispersed by an imaging spectrometer, and the intensity (as a function of wavelength) was measured on a CCD. Temperature determined fitting the spectral intensity to Wien's approximation to Planck's law.

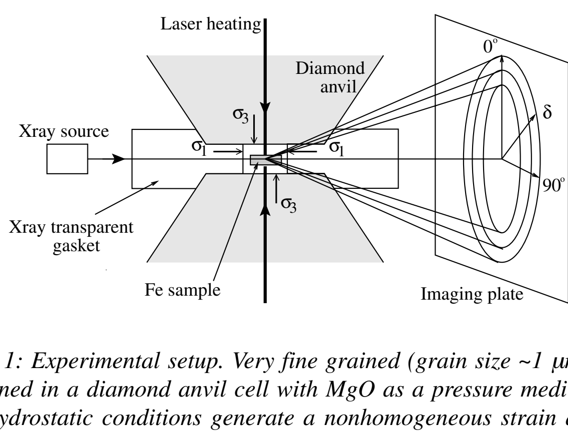

FIG. 1: Experimental setup. Very fine grained (grain size ~1 µm) Fe is confined in a diamond anvil cell with MgO as a pressure medium. The nonhydrostatic conditions generate a nonhomogeneous strain and texture in the sample. Laser heating of the sample was performed through the diamond anvils. The monochromatic x-ray beam was sent though the amorphous boron and epoxy gasket and collected on an imaging plate. The variation of the d-spacings and intensities of the diffraction peaks as a function of the azimuthal angle δ are controlled by the elasticity and texture in the sample.

Results and Discussion

For each pressure and temperature, we extracted the diffraction intensities for four peaks (100, 002, 101, 110) and 56 sample orientations with the azimuth angle on the imaging plate δ varying from –110º to 110º in 4º intervals. Intensities were integrated over the peak width in 2θ and the background was subtracted.

Figure 2 presents the variation of the intensity of diffraction for the Fe(002) peak as a function of the angle ψ between the dif-

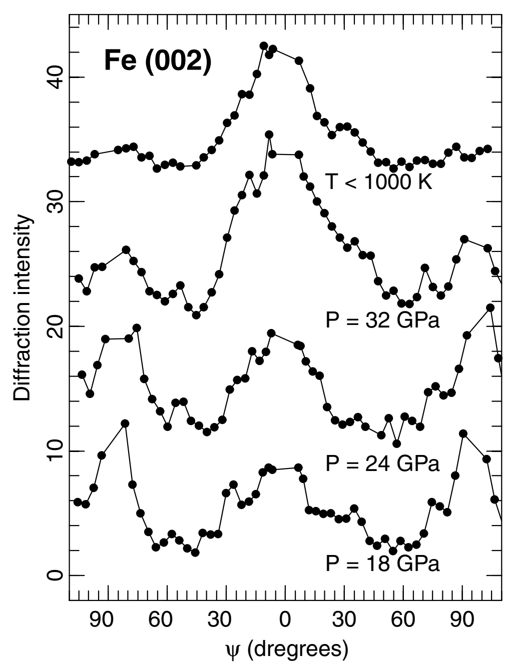

FIG. 2: Variation of the intensity of diffraction of the (002) line of ε-Fe as a function of the angle ψ between the diffracting plane normal and the load axis for selected pressures and temperatures.

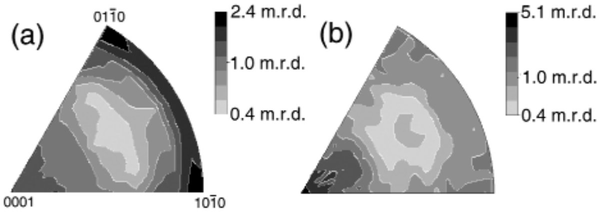

FIG. 3: Inverse pole figures illustrating preferred orientation patterns for ε-Fe deformed on axial compression at (a) P = 18 GPa and T = 300 K and (b) P = 32 GPa and T = 300 K. The maximum pole density is 2.39 multiples of a random distribution (m.r.d.) at 18 GPa, and 5.11 m.r.d. at 32 GPa.

fracting plane normal and the load axis for 18, 24, and 32 GPa while heating the sample to temperatures below 1000 K from 32 GPa and 300 K. After the transition to the ε phase, between 12 and 15 GPa, the *c*-axis of the crystallites are mostly orthogonal to the compression axis (peaks at ψ = -90º and ψ = 90º), whereas at higher pressures, the *c*-axis of the crystallites are mostly parallel to the compression axis (peaks at ψ = 0º); this does not change with increasing temperature.

From the intensity variation, the orientation distribution function was calculated. In the case of axial texture, the results can be represented as inverse pole figures for the direction of the diamond anvil cell axis (Fig. 3). Both diagrams show a strong preferred orientation with a dominating (0001) fiber component at the highest pressures (Fig. 3b).

These figures can now be used to study the deformation mechanisms and rheology of polycrystalline samples. This study also highlights new developments for performing quantitative texture analysis at high pressure and temperature.

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