Multigrain crystallography at megabar pressures

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High pressures produce complicated crystal structures. Single-crystal x-ray diffraction is the idea method for structure determination and refinement. However, the conventional single-crystal methods cannot be applied to a large number of submicron-sized crystals in the studies of phase transitions and chemical reactions at high pressure. Using a multigrain method for high-pressure samples, we have overcome this problem by sorting out crystallographic orientations of individual crystals [1]. In one rotation dataset obtained at megabar pressures, up to one thousand individual grains can be indexed applying the FABLE package [2]. Each grain can be treated as a single crystal [3]. The opening cone of a diamond anvil cell limits the possibility of performing wide omega rotations. We have further overcome this limitation by merging several grains with different orientations into one dataset and obtained high quality crystallographic data for seifertite SiO$_2$ at 129 GPa [4]. This development provides new opportunities for identification and characterization of unknown phases at megabar pressure and beyond.

Silica is one of the most abundant components on Earth. The phase transitions and structural evolution of SiO$_2$ with increasing pressure and temperature have been extensively studied over the past several decades. However, not until recently was the alumina-rich NiAs-type silica identified applying the multigrain diffraction method in a H$_2$O-bearing oceanic crust component under deep lower mantle conditions [5]. The presence of H$_2$O changes the stability of silica phase that coexist with bridgmanite in oceanic crust component subducted to the deep lower mantle (Fig. 1). The stability and chemical composition of mineral phases have to be demonstrated in realistic multicomponent compositions representative of the Earth system.

Multigrain diffraction methods in combination with ex situ chemical analysis on samples recovered to ambient conditions have showed great advantages in characterization of unknown phases in a multiphase assemblage at multigrain pressures. The advancement of the analytical techniques further allows us to study the effects of H$_2$O on the phase assemblages [6]. Knowledge of the mineralogy and chemical composition of lower mantle multicomponent systems, dry or wet, can be used to place constraints on the geochemical and geophysical models of the deep Earth.

![Figure 1](image_url)

**Figure 1.** The presence of H$_2$O determines the stability of silica phase and affects the chemical composition of coexisting bridgmanite. Coexistence of bridgmanite (Brd) and NiAs-type silica (Nt) was observed in experimental simulations of water-rich subduction at conditions corresponding to about 2,000 km depth of the lower mantle [5].


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