



Review article

In situ determination of crystal structure and chemistry of minerals at Earth's deep lower mantle conditions

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Abstract

Recent advances in experimental techniques and data processing allow in situ determination of mineral crystal structure and chemistry up to Mbar pressures in a laser-heated diamond anvil cell (DAC), providing the fundamental information of the mineralogical constitution of our Earth's interior. This work highlights several recent breakthroughs in the field of high-pressure mineral crystallography, including the stability of bridgmanite, the single-crystal structure studies of post-perovskite and H-phase as well as the identification of hydrous minerals and iron oxides in the deep lower mantle. The future development of high-pressure crystallography is also discussed.

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1. Introduction

Pressure, temperature and chemical composition (P – T – X) determine the phase diagrams, accounting for the material diversity of nature. These three dimensions are strongly correlated in geophysical and geochemical studies. Our knowledge of Earth's constitution is built on experimental measurements and theoretical simulations of the physical properties of minerals at high P – T conditions in comparison with seismic models [1,2]. Of all the properties, crystal structure and chemistry provide fundamental information, such as atomic arrangement and elemental partitioning of individual minerals in deep Earth.

Accurate determination of high-pressure mineral structure is crucial for understanding all other pressure-induced

property changes in the deep Earth. Polycrystalline structural refinement provides limited information about crystal structure, and single-crystal X-ray diffraction (XRD) will be the ideal method for structural determination. However, crystallography under deep-Earth conditions has been limited to polycrystalline samples because single crystals are unachievable in phase transition studies at ultrahigh pressures. This problem has been overcome by sorting out hundreds of sub-micron crystallites, and refining the structure of several selected crystallites [3,4].

2. Crystal structure and chemistry of silicates in the D'' region

At a depth of ~2890 km in the Earth's deep interior, the slowly convecting, highly viscous mantle silicates meet the liquid metals of the outer core. A thermal boundary is generated at the core-mantle boundary (CMB) where the temperature steeply increases to nearly 4000 K at the boundary of the core [5]. Seismic observations show that

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approximately 100–350 km above the core-mantle boundary, the so-called D'' layer presents a number of enigmatic features. These seismic anomalies in the D'' boundary include the D'' discontinuity, S wave polarization anisotropy, anticorrelated seismic velocity anomalies, and ultralow velocity zones (ULVZ) [6,7]. Sidorin et al. speculated that several intriguing seismic observation in the D'' layer can be explained by a solid–solid phase transition with a positive P/T slope of the boundary (Clapeyron slope) [8]. In 2004, Murakami et al. discovered the bridgmanite to post-perovskite transition in magnesium silicate (MgSiO_3), the dominant mineral in Earth's mantle [9]. Many significant predictions and experimental results have been achieved on this phase transition by the geological community, providing one valid interpretation of the seismological observations in the D'' region. However, recent observations of several abrupt increases in seismic velocity cannot be explained by a simple model of an iso-chemical MgSiO_3 phase transition from bridgmanite to post-perovskite, suggesting the possibility of compositional variations in the deep mantle [10].

2.1. Structural changes through bridgmanite to post-perovskite transition

The phase transition from bridgmanite to post-perovskite was observed experimentally in a polycrystalline sample above 125 GPa and 2500 K in a laser-heated DAC, as shown in Fig. 1 [9]. Here, we focus on the crystal structure and chemistry of bridgmanite and post-perovskite, the two dominant minerals in the lower mantle. The powder diffraction pattern alone did not allow unambiguous structure determination of the newly observed phase. The crystal structure of the post-perovskite was then predicted by theoretical calculations, which revealed the CaIrO_3 -type structure with space group $Cmcm$ [9,11,12].

CaIrO_3 -type MgSiO_3 post-perovskite adopts a 2D structure with edge- and corner-sharing SiO_6 octahedra arranged in linear chains along a and c axes, respectively (see Fig. 2). These edge- and corner-sharing SiO_6 octahedra sheets are alternated with interlayer Mg^{2+} ions along b axis (see Fig. 2). However, MgSiO_3 bridgmanite crystallizes in a 3D network structure with only corner-sharing SiO_6 octahedra. Because of the fundamental differences in crystal structures between bridgmanite and CaIrO_3 -type post-perovskite phases, first-principle calculations have predicted that the bridgmanite to post-perovskite transition has extraordinary property changes that may account for the large seismic anomalies observed in the D'' region [11].

Existing models of a bridgmanite dominant lower mantle have been built on the assumption that the atomic ratio $\text{Fe}/(\text{Fe} + \text{Mg})$ is nearly 0.1 in the entire lower mantle and a small percent of Al_2O_3 can be incorporated into the silicate phase [2]. The most abundant silicate mineral in Earth is Mg-silicate bridgmanite with 5–10 mol% of Fe and Al existing from 660-km depth to the D'' region. Bridgmanite can be synthesized above 20 GPa and ~ 1000 K in a multianvil apparatus and single crystals with a size of 10–100 μm can be recovered to ambient

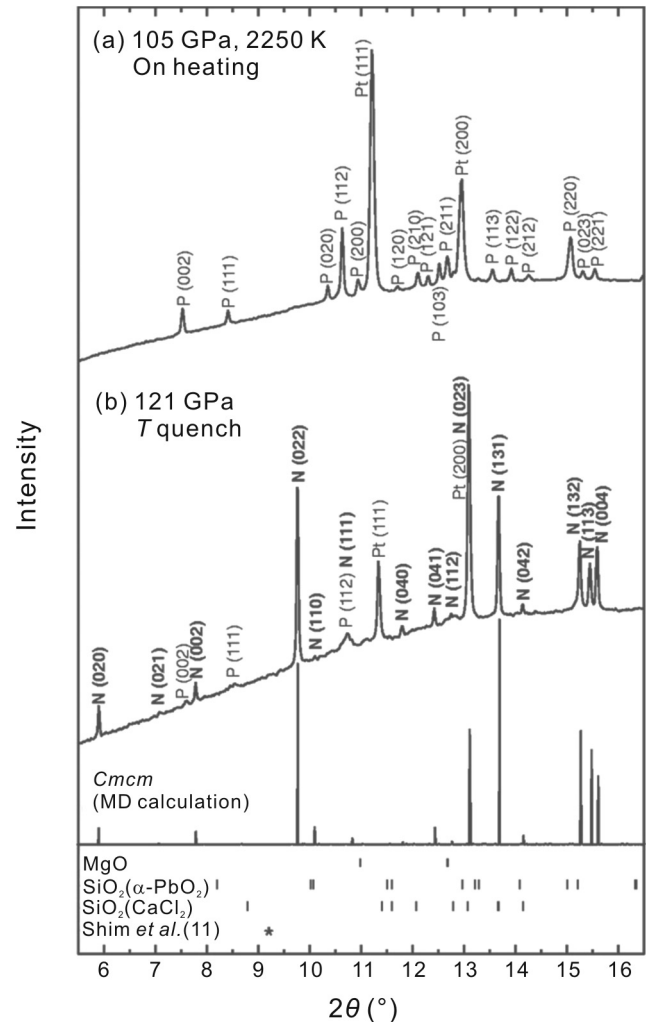


Fig. 1. XRD patterns of MgSiO_3 at (a) 105 GPa and 2250 K, (b) 121 GPa and 300 K after heating at 127 GPa [9]. Definitions are P, $Pbnm$ perovskite; Pt, platinum; N, new phase (post-perovskite). The calculated powder XRD pattern of the post-perovskite is shown for comparison. The small ticks indicate the peak positions of MgO and both $\alpha\text{-PbO}_2$ -type and CaCl_2 -type SiO_2 .

conditions for detailed structural studies. As a result, the effects of Fe^{2+} , Fe^{3+} and Al^{3+} on the bridgmanite have been extensively studied by various research groups [13–18]. In contrast, post-perovskite structure is unquenchable, and in-situ high P – T XRD experiments are essential to understand the structure–property relation [19–21]. Seismological observations show that the depth extent (or sharpness) of the D'' seismic velocity discontinuity is less than 75-km, corresponding to the pressure of <4 GPa [22–24]. However, in-situ high P – T experiments find that substitution of Fe and Al in MgSiO_3 bridgmanite tends to expand the transition over a much broader pressure range [25]. Considering strong thermal and chemical heterogeneities in the D'' layer, improved constraints from both seismology and mineral physics are needed [22].

Interestingly, interaction between the lowermost mantle and the liquid outer core may lead to an increased incorporation of Fe content into the D'' region [26,27]. Yamanaka et al. performed powder XRD Rietveld analysis on Fe-rich ($\text{Mg}_{0.6}\text{Fe}_{0.4}$) SiO_3 post-perovskite, suggesting a structure with the $Pmcm$

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