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Femtosecond diffraction studies of shock-compressed silicate melts at the LCLS-XFEL

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Abstract

SiO_2 is one of the most fundamental constituents in planetary science, being vastly abundant in the Earth's crust and mantle and free SiO_2 can be expected in localized regions in the Earth's mantle, derived from e.g. subducted oceanic crust [1]. The stability of SiO_2 within these regions is affected by polymorphism at high pressures and SiO_2 serves as an archetype for the dense highly coordinated silicates of planetary interiors and large (1-10M$\oplus$) exoplanets [2]. Seismological heterogeneities in the ultralow velocity zones (ULVZs) at the upper end of the transition zone and at the core mantle boundary (CMB) have been interpreted with the presence of higher coordinated SiO_2 melts [3][4]. We carried out time-resolved X-ray diffraction studies of silicon dioxide (SiO_2) at megabar pressures, using the long-pulse laser and shock diagnostics at the MEC end-station of the Linac Coherent Light Source (LCLS), USA. Our study mainly focused on the in-situ investigation and determination of Si-O coordination and bond length in silicate melts, and consequently, its structure factors and radial distribution.

1. Introduction

At ambient conditions, polymerized silicate melts are characterized mainly by networks of Si-O tetrahedra with a 4-fold coordination [5]. At 7 GPa, SiO_2 crystallizes in the tetragonal rutile-type structure (space group P42/mnm), which consists of slightly distorted SiO_6 octahedra that share edges to form chains running parallel to the c-axis [6]. In recent diamond anvil studies it was shown, that the change in coordination of silicate glass at ambient temperatures up to pressures of 50 GPa is a continuous process, with a reorganization of <Si-O> bond structure from 4- to 6-fold, and between 50 to 172 GPa from 6- to 6.8-fold [7]. Moreover, in dynamic experiments based on time-resolved shock compression of SiO_2 glass it was shown, that <Si-O> bond distance of 1.58 Å at ambient pressures is consistent with a 4-fold coordination. By comparison, shock recovered material from 33.6 GPa showed a <Si-O> bond distance of 1.68 Å, corresponding to a mixture of 4 to 6 coordination [9]. Further experiments on SiO_2 glass indicated, that changes in the Si-O coordination number from 4 to 6 occur at the same pressures in which the acoustic wave velocity changes [10]. However, structural changes that silicate glasses undergo cannot be assumed to be a completely valid model for silicate melts. Moreover, structural changes for SiO_2 melts at ultra-high pressures and temperatures from e.g. tetrahedral to octahedral Si-O networks could so far not be studied, despite their relevance to planetary models. Through laser induced shock compression and XFEL diagnostics, we were able to reach the liquidus conditions of SiO_2 and gain information about its phase transformations and melt structure.

2. Methods

Laser induced shock compression of amorphous and crystalline SiO_2, fused silica and quartz respectively, were investigated via transmission in-situ XRD at the Matter in Extreme Conditions (MEC) end-station of the Linear Coherent Light Source (LCLS), USA. Femtosecond hard X-rays pulses with photon energies of 11.2 keV were used to investigate the lattice level structure of SiO_2 during shock compression. A frequency doubled Nd:YAG glass laser pulse with a 10 ns pulse duration, and a top hat pulse shape launched a shock wave through the sample by creating a plasma on an plastic (kapton) ablator, which sent a shock wave into the sample due to mass and energy conservation, resulting in high densities and temperatures along its respective Hugoniot. While the sample material was compressed, LCLS X-Rays (SASE mode) were probing the sample at different time delays with regard to the laser pulse resulting in time-resolved X-Ray diffraction of the lattice level structure during compression of the sample. The X-ray diffraction data in this study includes a series of time delays, to investigate a change and transformation of the atomic structure of SiO_2 during the shock transit.

3. Results

This study shows, that quartz is shock transforming to stishovite at 25 GPa remaining in this phase up to 109 GPa, well within its liquidus regime. This so-called **superheating** was detected with the use of XRD. Melt of quartz was ultimately detected at 127 GPa, while time delays prior to these conditions showed metastable phases in the form of the $CaCl_2$ structure. Densities were measured from 3.2 g/cm^3 up to 5.03 g/cm^3 through d-spacing and impedance matching. By changing the shock direction of the quartz from z-cut to a-cut, significantley higher densities at same conditions were achieved (Fig. 1). Fused silica shows similar behavior to quartz, with a phase transformation to stishovite at 43 GPa remaining in this structure up to 64.5 GPa, well within its liquidus, therefore also indicating superheating behaviour. Shock melt of fused silica was then achieved at 88.5 GPa.

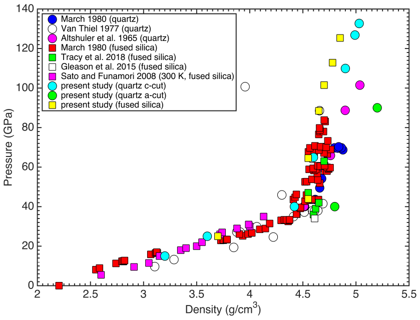

Figure 1: Density-pressure plot of SiO_2 obtained through gas-gun and laser shock experiments.

4. Summary and Conclusions

In this study we investigated laser induced shock compressed SiO_2 melts at high pressure with the use of an XFEL. We could show the phase transition of crystalline SiO_2 (quartz) to stishovite, to the $CaCl_2$ structure in a superheated state and ultimately the quartz melt structure. Similar behaviour was detected for fused silica, which transformed to crystalline stishovite, remaining in this structure even in its liquidus regime. This data will provide more information about lattice level structure of silicate melts, which eventually help to understand the evolution, interiors and dynamics of terrestrial planets.

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