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High pressure elastic and plastic deformations of silica: In situ diamond anvil cell Raman experiments

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Abstract

Normal silica glass is usually referred to as low density amorphous silica as it can be converted to high density amorphous silica by a hydrostatic pressure (polyamorphic transition). In this work in situ Raman experiments are performed in a diamond anvil cell up to 18 GPa. The pressure effects on the structure of silica after successive compression decompression experiments are analyzed. The mode Grüneisen parameters corresponding to the elastic compression of high density amorphous silica are obtained and compared with those of normal silica. A reorganization of the high density amorphous silica below 3 GPa is evidenced.

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1. Introduction

Silica is one of the most abundant components of the earth and one of the more extensively studied; however, its structural transformation under high pressure is not yet fully understood [1].

The observation of external perturbation effects affords to get a better understanding of the structure of silica. Temperature dependence has been extensively studied [2] and high pressure effects were mainly analyzed through Raman, infra-red or Brillouin experiments [3–8] or simulations [9–16]. Recent works, where densification effects are observed in indented silica [17], have motivated in situ high pressure Raman experiments in order to document the structural reversible and irreversible polymorphic transitions of silica glass. The structural reversible transition corresponds to an elastic behavior whereas the irreversible transition to an inelastic behavior.

Raman spectroscopy has been used mainly to characterize permanently densified samples recovered from high pressure measurements [5,7,13]. In situ measurements were also performed by Raman or Brillouin scattering [3,4,6,8]. However, in these experiments the analyzes were mainly focused on the strongest band (≈450 cm^{-1}) and no Raman data are available for successive compression and decompression experiments. These effects were, however, considered in recent molecular-dynamics simulations [15,16].

In this paper, we show the effects of compression and decompression cycles on the different Raman bands of silica in the range of pressure corresponding both to the elastic and plastic deformations and determine the mode Grüneisen parameters of high density amorphous silica in those pressure domains.

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2. Samples and experiments

The silica samples used in these experiments correspond to a Herasil quality (maximum 150 ppm OH contents). A silica sample was crushed in a pestle and one of the obtained ‘grain’ (typical size of $20 \times 70\ \mu m^2$) was meticulously introduced by the tip of a needle in the 200 μm diameter gasket hole of a diamond anvil cell.

The experiments were carried out in a diamond anvil cell (DAC), Sidoine model (Laboratoire de Physique des Milieux Condensés, Paris).

The pressure in the DAC was determined from the spectral shift of the ruby chips emission using methanol as pressure transmitting medium. Methanol is not considered as a hydrostatic medium up to 18 GPa [18] but the non hydrostaticity is limited as no significant fluorescence lineshape broadening is observed on the ruby emission up to 16 GPa. Indeed, a broadening of the linewidth is observed from 16 GPa.

The Raman spectra were recorded in situ with a Renishaw RM 1000 microspectrometer with a Ar^+-ion 514 nm, 50 mW laser excitation.

Successive compression, decompression and a second compression cycle were performed on the sample without unloading the cell: this insures the same conditions for the second compression run.

The Raman shifts for the different lines were observed in two different experiments. The first corresponds to a loading up to 8.6 GPa and the second to a loading up to 18 GPa followed by a decompression to 1 GPa and a new compression up to 16 GPa. At this point, the pressure was quickly released (breakage of a diamond anvil) and the Raman spectra of the retrieved sample were recorded at ambient pressure after 1 day.

3. Results

The first series of compression and decompression experiments is carried up to different maximum pressures of 8.5 and 9 GPa in the reversible domain in order to observe the transition between the elastic and plastic deformation domains. Fig. 1 shows a typical Raman spectrum at 8.6 GPa. Fig. 2 plots the shift of the main Raman lines for different pressures carried both in compression and decompression. The errors on the measurements and the determinations of the maximum of the main band, of the D_1 line and D_2 line are estimated to $\pm 1.0\ cm^{-1}$, 0.4 and $0.4\ cm^{-1}$, respectively. The plots size on Figs. 2(a) and (b) and 4(a) and (b) are larger than the estimated error bars. Concerning the $800\ cm^{-1}$ band, ω_4 (see Fig. 2(c)) the error is larger due to a broad band and is estimated to $\pm 3.0\ cm^{-1}$. The Boson peak, not observable with the Raman set up used, the $1200\ cm^{-1}$ and the $1060\ cm^{-1}$ silica bands, superimposed on the methanol line, will not be discussed in this paper. The slopes of the curves for the main band at $\omega_1 = 450\ cm^{-1}$, the D_1 line at $\omega_2 = 490\ cm^{-1}$, the D_2 line at $\omega_3 = 607\ cm^{-1}$ and the band at $\omega_4 = 800\ cm^{-1}$ are, respectively,

$$\left(\frac{\partial\omega_1}{\partial P_1}\right) = 10.4 \pm 0.8\ cm^{-1}/GPa,$$

$$\left(\frac{\partial\omega_2}{\partial P_1}\right) = 5.2 \pm 0.2\ cm^{-1}/GPa,$$

$$\left(\frac{\partial\omega_3}{\partial P_1}\right) = 1.5 \pm 0.1\ cm^{-1}/Gpa,$$

$$\left(\frac{\partial\omega_4}{\partial P_1}\right) = 8.4 \pm 0.9\ cm^{-1}/GPa.$$

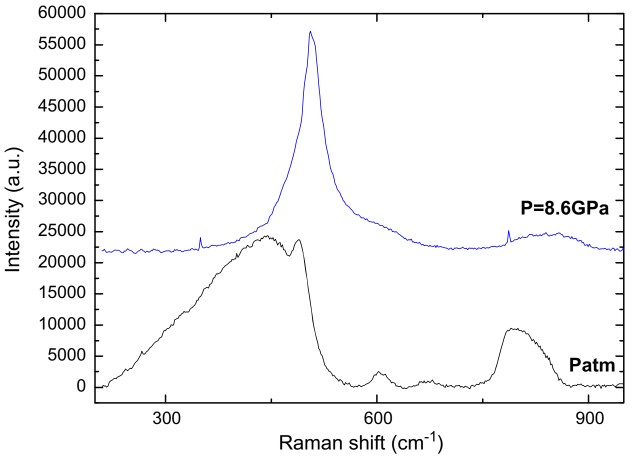

Fig. 1. Raman spectra of non densified silica glass (at 0 GPa) and at pressure 8.6 GPa (elastic domain).

For the ω_4 band which clearly includes at least two components (Fig. 1), we plot the position of the maximum of the band without deconvolution.

During the second series of experiments, with compression pressures above 9 GPa, silica deformation is no longer elastic. The Raman spectra of the recovered materials are different from those of the original SiO_2 glass, corresponding to an irreversible domain. Fig. 3 shows the in situ Raman spectra for the glass at 18 GPa and for the recovered sample measured at ambient pressure after the second compression. Fig. 4(a) shows the plot of the positions of the main band ω_1 and of the D_1 line for a complete cycle: a first compression up to 18 GPa followed by a decompression down to 1 GPa and a second compression up to 16 GPa and a quenching at ambient pressure. The Fig. 4(b) and (c) is the corresponding plots recorded in the same cycle for the D_2 line and for the $800\ cm^{-1}$ line. The slopes during the second compression, in the linear part between 3 and 16 GPa, are respectively,

$$\left(\frac{\partial\omega_1}{\partial P_2}\right) = \left(\frac{\partial\omega_2}{\partial P_2}\right) = 4.5 \pm 0.2\ cm^{-1}/GPa,$$

$$\left(\frac{\partial\omega_3}{\partial P_2}\right) = 1.3 \pm 0.1\ cm^{-1}/GPa,$$

$$\left(\frac{\partial\omega_4}{\partial P_2}\right) = 3.7 \pm 0.4\ cm^{-1}/GPa.$$

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