Physics of the Earth and Planetary Interiors 233 (2014) 95–102

Contents lists available at ScienceDirect

Physics of the Earth and Planetary Interiors

journal homepage: www.elsevier.com/locate/pepi

Differential stress effect on the structural and elastic properties of forsterite by first-principles simulation

Lei Liu *, Jianguo Du, Hong Liu, Li Yi

Key Laboratory of Earthquake Prediction, Institute of Earthquake Science, China Earthquake Administration, No. 63 Fuxing Road, Haidian District, Beijing, China

ARTICLE INFO

Article history:
Received 9 August 2013
Received in revised form 11 May 2014
Accepted 5 June 2014
Available online 18 June 2014

Keywords:
Differential stress
Structural parameters
Elastic properties
Forsterite
First-principles simulation

ABSTRACT

To understand the effect of differential stress on the properties of forsterite, changes of its structural parameters and elastic properties under different differential stress were calculated by first-principles simulations. Totally, 5 sets of different stresses results (namely $x = 0$, ±1 and ±2 GPa, x is the stress difference among σ_{zz}, σ_{yy} or σ_{xx}), were calculated. The effect of differential stresses on lattice constants show Poisson effect. Compared with the results under hydrostatic stress, all lattice strain (ε_a, ε_b, and ε_c) significantly increased at differential stress conditions. Furthermore, when the largest differential stresses are positive they more effect on lattice strain than the differential stresses are negative. Effect of different differential stress on density of forsterite is different. Compared with the density under hydrostatic pressure, positive differential stresses applied in the x direction or negative differential stresses applied in the y direction make forsterite density decreasing; however, positive differential stresses applied in the y direction or negative differential stresses applied in the x direction make forsterite density increasing. The density differences caused by differential stress are close to the upper mantle density anomaly. The effect of differential stress on density and lattice parameters is more notable when the absolutely value of $\Delta\sigma_{xx}$ or $\Delta\sigma_{yy}$ are the biggest among the differential stresses, namely stresses distributing along a and b axis orientation are more influenced on forsterite structural parameters than c axis orientation. Full elastic constants, bulk and shear modulus of forsterite (C_{11}, C_{22}, C_{33}, C_{44}, C_{55}, C_{66}, C_{12}, C_{13}, C_{23}) were calculated under different stress conditions. Bulk modulus, shear modulus and elastic constants of differential stress are also different with the values at hydrostatic pressure, but the calculated results do not show any significant trends.

1. Introduction

Differential stress commonly exists in the crust and mantle of the Earth. The average differential stress in the upper crust around the San Andreas fault was estimated to be 50 MPa, which affected the strength of the fault (Fialko et al., 2005). Experiments on quartz fabrics under differential stress have shown that Raman spectra at different sites of the deformed samples are different indicating that the differential stress changes their crystal structures (Ma et al., 2009). In addition, differential stress could affect the development of olivine lattice preferred orientation (LPO) (Nicolas et al., 1973; Zhang and Karato, 1995; Bystricky et al., 2000; Warren et al., 2008). Constraining the variation in olivine LPO produced under shear conditions is the key to interpreting seismic anisotropy in the mantle.

Orthosilicate olivine ($(Mg,Fe)_2SiO_4$), is considered to be one of the main constituents of the upper mantle. At low temperatures, the differential stress in the olivine crystal is very high (Chen et al., 2004; Raterron et al., 2004), and can reach upto 5 GPa at ~100 °C (Evans and Goetze, 1979). The differential stress in the olivine crystal at 8 GPa and 820 °C increases as the main stress increases from ~0.6 GPa to 1.7 GPa (Li et al., 2004). Measurement of the San Carlos olivine at pressures of 3–5 GPa and temperatures of 25–1150 °C indicates that the differential stress in olivine at temperatures lower than 900 °C is 2.5 GPa; however, it drastically decreases to ~1 GPa and is temperature dependent if the temperature is higher than the transition temperature (900 °C) (Long et al., 2011).

Although considerable experimental studies on olivine properties under the condition of differential stress (or shear stress) have already been conducted, the structural and elastic parameters as a function of the differential stress are rarely reported. Following the development of computer technology, first-principles calculations

* Corresponding author. Tel.: +86 1088015473.
E-mail addresses: liulei@seis.ac.cn, lerry00@sina.com (L. Liu).

http://dx.doi.org/10.1016/j.pepi.2014.06.010
0031-9201/

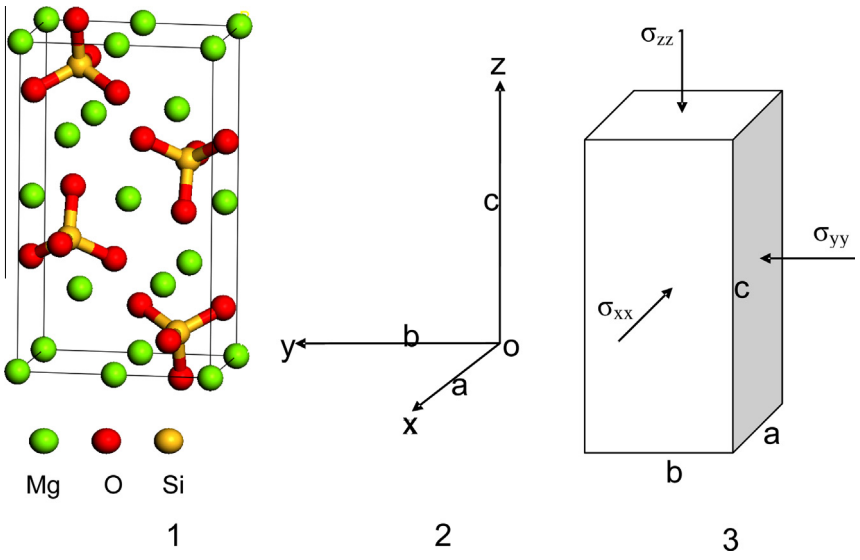

Fig. 1. Atomic structure of forsterite and schematic diagram of differential stress project. (1) Atomic structure of forsterite, (2) lattice constants and directions, and (3) applied stresses (σ_{xx}, σ_{yy}, and σ_{zz}).

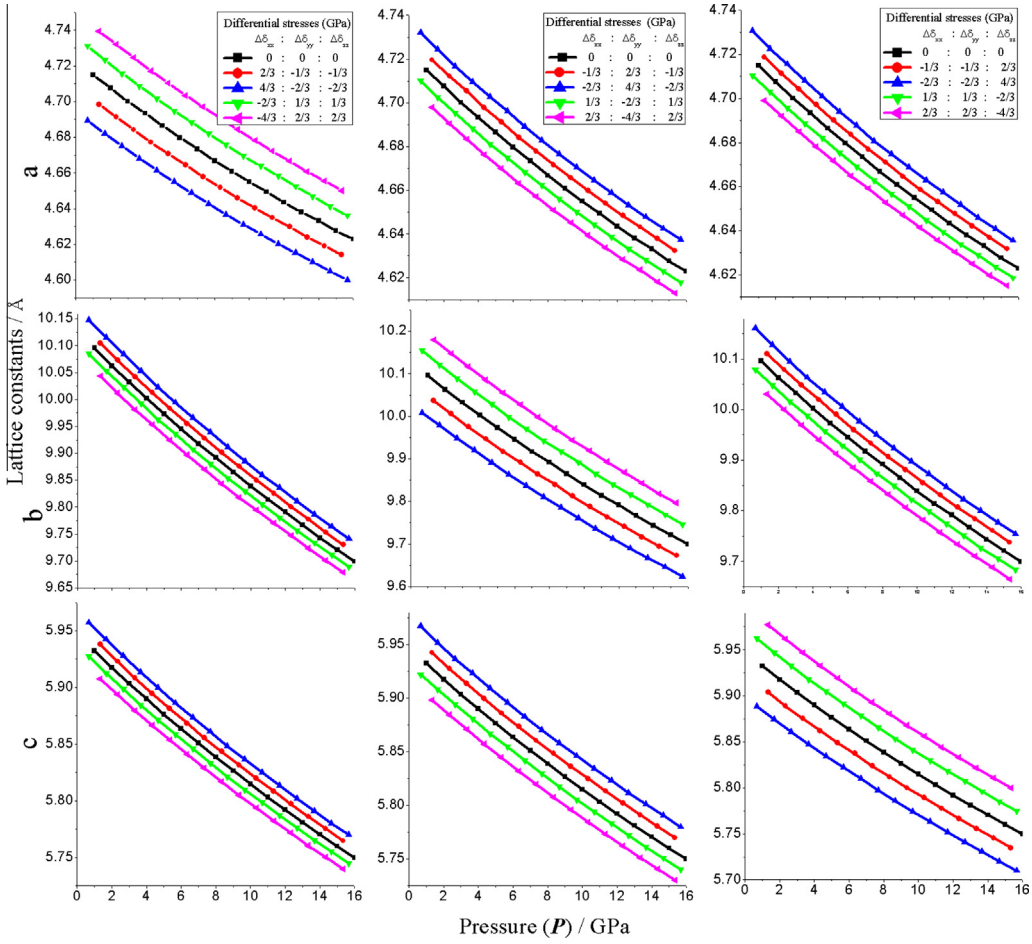

Fig. 2. Changes of lattice constants with pressure.

based on the density functional theory (DFT) have been successfully applied to the simulation of mineral properties (Gillan et al., 2006; Wentzcovitch et al., 1993; Karki et al., 2001; da Silva et al., 1997). In this study, the structural and elastic parameters of forsterite (Mg_2SiO_4), the magnesium-rich end-member of olivine, were calculated by a first-principles method at high pressure to understand the structural changes in forsterite under differential stress.