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Formation and properties of water from quartz and hydrogen at high pressure and temperature



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ABSTRACT

Quartz, as the most stable low-pressure polymorph of silica (SiO₂), is widely abundant in Earth's crust and mantle, exhibiting relatively high chemical stability. Although silica is only slightly soluble in water at ambient conditions, producing silicon-based weakly acidic compounds, Shinozaki et al. (2014) have shown recently that water itself can be formed by dissolution of SiO₂ in H₂ fluid under high- temperature and pressure conditions. Here, we have simulated this process via molecular-dynamics techniques based on a reactive force-field description of the SiO₂/H₂ interface. Diffusion of the H₂ fluid into the quartz crystal lattice was observed upon increasing temperature and pressure, followed by interaction of dissociated, atomic hydrogen with oxygen atoms in the SiO₂ lattice, disrupting the lattice and leading to the formation of water. Interestingly, water is evolved in the subsurface region of the silica, and it remains confined there, isolated from the hydrogen fluid, which corresponds precisely to the ice-like spectroscopic patterns observed experimentally. The over-pressured water formed from quartz and H₂ is a possible trigger for nucleating enigmatic deep earthquakes in the continental mantle lithosphere.

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1. Introduction

Silicon dioxide, known as silica, is, with its rich tapestry of various polymorphs and forms, one of the most abundant materials that can be found on Earth and other terrestrial planets. The stability and chemical reactivity of silica under ambient, as well as high- temperature and pressure conditions, are therefore of key interest not only to geoscience but also for wide industrial and technological applications. The phase diagram of silica, exhibiting polymorphism and assessing its thermodynamic stability, was completed relatively recently (Swamy et al., 1994) for temperatures up to 3200 K and pressures up to 15 GPa. In this high- temperature and pressure phase-diagram region, silica can metamorphose from quartz, the most stable form of SiO₂ at ambient conditions, to tridymite, cristobalite, coesite and stishovite. The first three polymorphs are well known for their low-temperature (α) and hightemperature (β) forms (Heaney, 1994 and Russell et al., 1994).

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Because of its ubiquitous presence and technological importance, properties of guartz have been widely studied both experimentally (Akaogi et al., 1995; Bourova and Richet, 1998; Lang et al., 1994; Levien et al., 1980) as well as by computer simulations (de Boer et al., 1996; de Leeuw et al., 1999; Skelton et al., 2011). Except for pH-dependent proton ad/desorption on the silica surface in aqueous environments (Fuerstenau and Pradip, 2005; Sulpizi et al., 2012), and low solubility in water (Anderson and Burnham, 1965; Morey et al., 1962), quartz is chemically a very stable material at ambient conditions, and generally does not interact with other species. Recently, Shinozaki et al. (2014) reported dissolution of SiO₂ in H₂ fluid under high pressure and temperature conditions relevant to Earth's upper mantle, which was studied by Raman and infrared spectroscopy. In contrast to aqueous dissolution, which leads to silicon species containing hydroxyl groups such as H₄SiO₄ or H₆Si₂O₇, dissolution in hydrogen gas at high pressure and temperature yields SiH₄ and H₂O. Here, in an effort to elucidate the underlying mechanisms of this interesting process, we carry out molecular-dynamics (MD) simulations to capture the essential underlying features, which are shown to have important implications for the origin of water on Earth to



Fig. 1. Snapshots of the silica slab in different stages of the performed MD simulation: (a) initial structure; (b) initial model equilibrated to T = 100 K and p = 1 GPa; (c) structure at T = 580 K and p = 1.3 GPa; (d) structure at T = 1220 K and p = 1.7 GPa; (e) final structure at T = 1700 K and p = 2 GPa. All structures are oriented to (100) direction. Silicon atoms are shown in green, oxygen in red and hydrogen in light blue color. (For interpretation of the colors in this figure, the reader is referred to the web version of this article.)

the nature of mantle dynamics and the trigger for nucleating deep earthquakes in the continental mantle lithosphere.

2. Computational details

We created a bulk model of α -quartz with a trigonal supercell (a = b = 29.460 Å, c = 64.824 Å, $\alpha = \beta = 90.0^{\circ}$, $\gamma = 120.0^{\circ}$) containing 1296 SiO₂ units. We relaxed this model by slow, gradual heating to 100 K and to a pressure of 1 GPa by NPT molecular dynamics (MD) simulation. The timestep for all MD used throughout this study was 0.2 fs. Analogously, we prepared the trigonal supercell of identical dimension filled by 3294 hydrogen molecules (H₂), and this model was equilibrated to the same state (100 K, 1 GPa) as the former one. The density of H₂ fluid was selected to conform to a pressure of 1 GPa at 100 K, using the virial definition in a single-phase calculation (Allen and Tildesley, 1989), prior to incorporation into this solid/liquid interfacial system. These two structures were merged to form an initial SiO₂/H₂ interfacial model – the quartz slab was separated by 1.5 Å from hydrogen fluid at both sides, resulting in initial z cell dimension of 147.0 Å. This system was then brought very carefully to a target temperature of 1700 K and a pressure 2 GPa (corresponding to experimental conditions, Shinozaki et al., 2014), by a sequence of 20 ps NPT-MD runs. To avoid any artificial structural changes, this sequence of NPT equilibration runs was divided into 10 stages. At each stage, the temperature was raised linearly by 160 K and the pressure by 100 MPa during each 20 ps simulation, where the thermal bath was coupled by a five-chain Nosé-Hoover thermostat-barostat (Jang and Voth, 1997; Martyna et al., 1992). We equilibrated the system by at least another 20 ps of MD at each stage, until thermodynamic quantities had converged. The system was successfully equilibrated at each stage, which was confirmed by subsequent short NVE simulations featuring excellent energy conservation and no substantial temperature drift; no unexpected structure changes or sudden potentialenergy jumps occurred.

MD was conducted with the reactive force field ReaxFF developed by van Duin et al. (2001, 2003), as implemented in the LAMMPS software package (Aktulga et al., 2012; Chenoweth et al., 2008; Plimpton, 1995). In contrast to conventional force fields, ReaxFF calculates bond orders and atom valences dynamically, based on the evaluation of many-body potential terms. The atomic charges were calculated by the charge-equilibration (QEq) algorithm, and thus they reflect the structural changes in the system. ReaxFF, therefore, allows description of chemical changes within an MD framework. The good performance of these reactive force fields for the silica/water interface was recently demonstrated by Fogarty et al. (2010).

3. Results and discussion

3.1. Formation of liquid water layer

Silica, in its α -quartz polymorph, is very stable at ambient pressure and room temperature when no interaction with molecular hydrogen can be expected. Therefore, we first performed MD of the SiO₂/H₂ interface under these conditions to confirm the stability of our model and performance of the reactive force field. Hydrogen gas at this temperature and pressure is very dilute, with an experimental density of 0.0899 g/cm³, behaving practically as an ideal gas; its contact with the silica surface is minimal. Naturally, silica undergoes structural relaxation near the surface, while the bulk region of the slab model maintains the regular crystal structure. As the surface model was created by cutting bulk quartz crystal, dangling bonds can be found on the surface atoms, the valence of which is not saturated chemically. This high-energy structure undergoes reconstruction when the surface layer is relaxed, and a fraction of the surface oxygen atoms interacts with hydrogen (Fig. 1a). Reconstruction causes increase of surface density as the first two SiO₂ layers merge together on most of the surface and form three- and six-membered ring as described in Rignanese et al. (2000). In particular, the six-membered rings are large enough to allow H₂ penetration into SiO₂ as discussed below.

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