Water diffusion in silica glass through pathways formed by hydroxyls

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ABSTRACT

Water diffusion in silicate melts is a fundamental process controlling physical and chemical consequences for magmatism, but mechanisms of diffusion in silicate glasses and melts are not fully understood. In this study, water diffusion experiments in silica glass were performed at temperatures of 650–850 °C and water vapor pressure of 50 bar, with the aim of improving our understanding of the mechanism of water diffusion in a simple SiO2–H2O system, and to construct a general water diffusion model for multi-component silicate glasses. Hydrogen diffusion profiles in silica glass were measured by secondary ion mass spectrometry (SIMS) down to a water concentration of ~10 ppm. Water diffusion profiles indicate that water diffusion becomes slower with decreasing water concentration in silica glass, with the water concentration dependence being greater than in multi-component silicate glasses, particularly at low concentrations (e.g., Doremus 1969, 2000; Zhang and Behrens 2000). A new water diffusion model is proposed for silica glass, where the greater concentration dependence is attributed to the limited number of diffusion pathways in silica glass, formed by breaking Si–O–Si bonds through hydroxyl formation. The model was applied to multi-component silicate glasses, taking into account the effects of metal cations that act as network modifiers by providing additional diffusion pathways for water molecules. The lower water concentration dependence in multi-component silicate glasses and melts is explained by little dependence of the number of diffusion pathways on water concentration because it is controlled extrinsically by network modifier cations. It is concluded that the number of diffusion pathways is an essential controlling factor for water diffusion in silica and silicate glasses.

Keywords: Water, diffusion, silica glass, SIMS, diffusion pathway

INTRODUCTION

Water is the most abundant volatile component of magmas. It changes various properties of silicate melts, for example, lowering the viscosity and melting temperature. In volcanic systems, water affects the eruption style through degassing and magma fragmentation due to bubble nucleation and growth in oversaturated ascending magma (e.g., Sparks 1978). Bubble growth in magma is controlled by viscous relaxation and water diffusion, the relative influences of which depend on magma properties such as temperature, pressure, and chemical composition. Water diffusion in silicate melts is thus one of the important basic parameters controlling the physical and chemical aspects of magmatism.

The diffusion of water in silicate glasses, as a potential analog of silicate melts, has been studied mainly in silica-rich glasses (e.g., Zhang et al. 2007 and references therein). Doremus (1969, 1995) concluded that water diffusivity in silica glass depends linearly on water concentration at 650–1000 °C, based on published data (Drury et al. 1962; Drury and Roberts 1963; Roberts and Roberts 1964, 1966; Burn and Roberts 1970). This dependence is consistent with that reported by Behrens (2010) for silica glass at 521–1097 °C at a total pressure of 2 kbar. Tomozawa and coworkers studied water diffusion in silica glass at relatively low water vapor pressures (e.g., Wakabayashi and Tomozawa 1989; Tomozawa et al. 1994, 2001; Davis and Tomozawa 1995; Oehler and Tomozawa 2004), and Wakabayashi and Tomozawa (1989) reported that water diffusion is independent of water concentration in silica glass at 400–600 °C and 0.5 bar. Regarding silica-rich glasses and melts, Doremus (2000) used literature data (Delaney and Karsten 1981; Karsten et al. 1982; Laphan et al. 1984) to show a linear concentration dependence of water diffusion in rhyolite melts at 650–1000 °C and a water vapor pressure of 0.7–5.0 kbar. Zhang and Behrens (2000) showed empirically that water diffusion depends exponentially on water concentration in rhyolite glasses and melts over wide ranges of both temperature and pressure (400–1200 °C and 0.01–8.1 kbar). Water diffusivities in rhyolite melts and silica glass exhibit a single Arrhenius relationship (Ni et al. 2015) even though their properties (e.g., structural relaxation) differ, implying that data on water diffusion in silicate glasses could potentially be applied to silicate melts with caution.

Many diffusion models have been proposed for water diffusion in silicate glasses and melts, but no universal model exists to describe the water diffusion in silicate glasses with various water concentrations and compositions. To elucidate the water