Melting curve of NaCl to 20 GPa from electrical measurements of capacitive current

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ABSTRACT

Using an in situ electrical method and the multi-anvil apparatus, we determined the melting curve of sodium chloride (NaCl) up to ~20 GPa, with an estimated uncertainty of ±40 K. Our results agree well with the existing data up to 6.5 GPa. At higher pressures, the melting temperatures from this study are as much as 200 K higher than those from an experimental study using the diamond-anvil cell (DAC), and are up to 500 K lower than those from theoretical studies using molecular dynamics (MD). The discrepancies may originate from surface melting in the DAC measurements, which underestimate the melting temperature, and from superheating in MD calculations, which over-predict the melting temperature. Fitting our results to the Simon equation yield \( \frac{T}{T_0} = \frac{P}{P_0} \cdot (P - P_0)^{1/3} \) where \( T \) and \( T_0 \) are the melting temperatures at \( P \) and \( P_0 \), respectively, with \( T_0 = 1073.6 \) K, \( T \) in K and \( P \) in GPa. The Simon equation fits the experimental data within uncertainties and therefore can be used to interpolate the melting curve. Using the equation of state (EoS) of NaCl at 300 K, the results are fitted to the Kraut-Kennedy equation in the form of \( \frac{T}{T_0} = \left( V - V_0 \right) / V_0 = 4.37 + 1 \), where \( T \) (in K) and \( T_0 = 1073.6 \) K are the melting temperatures at \( V \) and \( V_0 \) (at 0.001 GPa), respectively. At pressures above 14 GPa, the experimental data deviate from the Kraut-Kennedy equation fit toward lower temperatures, probably because the volume dependence of the Grüneisen parameter was ignored in the equation. The Gilvarry-Lindemann equation \( T_{m0} \sim 1.698 \cdot \frac{f^2}{\Theta} \left( \frac{V_0}{V} \right)^\gamma \) provides a satisfactory fit to the melting curve of NaCl between 0 and 19 GPa if the exponent \( q \) in the volume dependence of the Grüneisen parameter \( \gamma = \gamma_0 \left( V/V_0 \right)^q \) is allowed to deviate from one. Given that the melting curve of NaCl up to 6.5 GPa is well established, monitoring the melting of NaCl offers an efficient alternative for pressure calibration of large-volume high-pressure apparatus for Earth science applications.

Keywords: Melting curve, high pressure, capacitive current, in situ electrical method, sodium chloride, Simon equation, Kraut-Kennedy equation, Lindemann’s law

INTRODUCTION

Melting plays a critical role in planetary differentiation and dynamics. Knowledge of the pressure-dependent melting temperatures of Earth materials is of fundamental importance for constraining the Earth’s thermal structure, understanding geochemical cycles, and interpreting seismic observations (Boehler 1996). Many experimental methods have been developed to investigate melting at high pressure. As a first-order phase transition, melting is characterized by the loss of long-range atomic order, which manifests as the disappearance of reflections from lattice planes and appearance of diffuse scattering signal in X-ray diffraction patterns (Anzellini et al. 2013). Melting is associated with significant changes in lattice dynamics, which lead to vanishing Lamb-Mössbauer factor (Jackson et al. 2013). The latent heat of melting gives rise to enhanced absorption of heating power (Boehler et al. 1997; Lord et al. 2009) and may be detected through differential thermal analysis (DTA) (Akella et al. 1969). Furthermore, melting results in loss of shear strength and precipitous reduction in viscosity, which can be detected through textural change (Boehler et al. 1997; Chen et al. 2008), from the sinking of a dense sphere marker (Dobson et al. 1996), or from discontinuous change in electrical resistivity (Brand et al. 2006). Measuring the melting temperatures of materials at the pressure conditions of deep Earth poses considerable technical challenges and consequently experimental data are limited and often uncertain (e.g., Anzellini et al. 2013; Boehler 1996; Shen and Lazor 1995).

As a simple ionic compound, sodium chloride (NaCl) has been investigated extensively in an attempt to gain insights into its melting mechanism and melt structure (e.g., Clark 1959; Boehler et al. 1997; An et al. 2006). In high-pressure research, NaCl is widely used as a thermal insulating material and pressure marker in diamond-anvil cell (DAC) experiments, and therefore knowledge of its melting curve helps to assess its applicable ranges of pressure and temperature (e.g., Shen et al. 2001). Furthermore, monitoring the melting of NaCl offers an appealing alternative for pressure calibration of large-volume apparatus such as the piston-cylinder apparatus and multi-anvil press (e.g., Leinenweber et al. 2012), with several advantages including: (1) melting occurs much more rapidly than solid-state phase transition; (2) melting can be readily recognized using a sinking marker such as a Pt sphere; and (3) high-purity NaCl is readily available and less expensive than gold, the melting curve of which has been used for pressure calibration.

Earlier studies have determined the melting curve of NaCl...