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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 (NaC1) 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 $(T/T_0)^{4.5} = (P - P_0)/0.6 + 1$, 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 $T/T_0 = (V_0 - V)/V_0 \cdot 4.37 + 1$, where T (in K) and T_0 (= 1073.6 K) are the melting temperatures at V and V_0 (at 0.0001 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 $T_m \sim 1.689 \cdot f^2 \cdot \Theta_0^2 \cdot (V_0/V)^{2(\gamma - 1/3)}$ 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 $\gamma = \gamma_0 \cdot (V/V_0)^q$ 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