

High-pressure X-ray diffraction study on the structure of NaCl melt using synchrotron radiation

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ABSTRACT

Molten NaCl was analyzed by high-pressure X-ray diffraction experiments using synchrotron radiation up to 5 GPa and 1600 °C along the melting curve. The interference function $Qi(Q)$ and the correlation function $g(r)$ were derived from the diffraction data. The first-neighbor distance r_1 is about 2.7 Å and the second-neighbor distance appears around $1.4r_1$ – $1.5r_1$. The coordination number, CN, of the nearest neighbor ions increases with pressure from 3.5 at 0.1 MPa to 4.5 at 5 GPa. This is the evidence that the NaCl melt has a B1-like structure with large vacancies over this pressure range and becomes densified by an increase in CN as a result of second neighbor compaction.