

American Mineralogist, Volume 84, pages 341–344, 1999

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

SATORU URAKAWA,¹ NAOKI IGAWA,² OSAMU SHIMOMURA,³ AND HIDEO OHNO³

¹Department of Earth Sciences, Okayama University, Okayama 700-8530, Japan

²Department of Material Innovation, Japan Atomic Energy Research Institute, Tokai 319-1195, Japan

³Spring-8, Japan Atomic Energy Research Institute, Mikaduki 679-5198, Japan

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.