

Phase transition in SiC from zinc-blende to rock-salt structure and implications for carbon-rich extrasolar planets

YUTO KIDOKORO^{1,2,*}, KOICHIRO UMEMOTO², KEI HIROSE², AND YASUO OHISHI³

¹Department of Earth and Planetary Sciences, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro, Tokyo 152-8551, Japan

²Earth-Life Science Institute, Tokyo Institute of Technology, 2-12-1 Ookayama, Meguro, Tokyo 152-8550, Japan

³Japan Synchrotron Radiation Research Institute, SPring-8, 1-1-1 Kouto, Sayo, Hyogo 679-5198, Japan

ABSTRACT

We have investigated the phase transition in SiC between the zinc-blende and rock-salt structures at high pressure and temperature in a laser-heated diamond-anvil cell. Results demonstrate that the transition occurs at 74 GPa and 2100 K with a 21% density increase, reflecting the coordination number rising from four to six. In addition, our ab initio calculations show that the boundary has a negative Clapeyron slope of -4.0 MPa/K at 2000 K. The experimentally determined phase boundary is located between those predicted by GGA and B3LYP functional. This transition may take place inside carbon-rich extrasolar planets, forming a boundary with a large density jump. Since SiC is rigid and highly thermally conductive, thermal convection in an SiC-dominant layer is not likely to occur. Nevertheless, the convection may be possible if planet interiors include both silicon carbide and silicate, and in this case the phase transition could affect the style of thermal convection.

Keywords: Silicon carbide, phase transition, zinc-blende, rock salt, Clapeyron slope, extrasolar planet