Thermal properties of close-packed Fe up to 400 GPa determined using Hugoniot functions YUKIO SANO, TOMOKAZU SANO, Osaka University — A quadratic equation for the temperature-independent Grüneisen coefficient γ was derived by a method in which the Walsh-Christian and Mie-Grüneisen equations are combined. Some previously existing *ab initio* temperature Hugoniots for hexagonal closed-packed solid Fe are inaccurate because the constant-volume specific heats on the Hugoniots C_{VH}, which are related uniquely to the solutions of the quadratic equation, have values that are too small. A C_{VH} distribution in the solid phase range was demonstrated to agree approximately with a previous *ab initio* distribution. In contrast, the corresponding γ distribution was significantly different from the *ab initio* distribution in the lower pressure region, and the γ distribution in the liquid phase range had a considerably larger gradient than the *ab initio* distribution. The causes of these disagreements are clarified. [Ref. Y. Sano and T. Sano, Phys. Rev. B 69, 144201 (2004).]

Tomokazu Sano
Osaka University

Date submitted: 04 Apr 2005

Electronic form version 1.4