Grüneisen parameter of $\varepsilon$-iron up to 300 GPa from in-situ X-ray study

L.S. Dubrovinsky,1,* S.K. Saxena,1† N.A. Dubrovinskai,1 S. Rekhi,1 and T. Le Bihan2

1Institute of Earth Sciences, Uppsala University, S-752 36 Uppsala, Sweden
2European Synchrotron Radiation Facility, Grenoble 38043, France

ABSTRACT

We show that high-quality powder X-ray diffraction data, collected in diamond anvil cells, provide sufficient information for Rietveld refinement and determination of temperature factors. For the first time using a new method based on combination of thermal equation of state and measured mean-square atomic vibrations of high-pressure $\varepsilon$-Fe phase, we determine Debye temperatures at pressure up to 300 GPa and temperature over 1000 K. We found that the Grüneisen parameter of $\varepsilon$-iron could be described by Anderson’s (1967) equation with parameters $\gamma_0 = 1.78(6)$, $q = 0.69(10)$ with fixed $V_0 = 6.73$ cm$^3$/mol.

INTRODUCTION

Iron is considered as the major component constituting the core of Earth. Therefore, the properties of iron at elevated pressure and temperature are very important to model the composition and dynamic of the core. The Grüneisen parameter $\gamma$ has been widely used to characterize and extrapolate the thermophysical properties of materials to high pressures and temperatures. Available data on the behavior of the Grüneisen parameter for iron under deep Earth conditions are limited and not in complete agreement with each other (Table 1). Anderson (1967) suggested the dependence of Grüneisen parameter on volume $V$ as follows:

$$\gamma = \gamma_0 \left( \frac{V}{V_0} \right)^q$$

(1)

where subscript 0 implies values at reference (ambient, if not another) conditions and $q$ is a parameter.

Boehler and Ramakrishnan (1980) measured $\gamma$ as function of pressure $P$ for $\alpha$-iron using the adiabatic decompression method and found $\gamma_0 = 1.66$ and $q = 0.6$. McQueen et al. (1970) provided the Grüneisen parameter to more than 100 GPa based on finite differences in thermal pressure between porous and non-porous Hugoniot data. They found $q = 1.0$ to be a reasonable approximation to their scattered data. Jeanloz (1979) reconsidered the same porous Hugoniot data and proposed that $q$ is equal to 1.62. Brown and McQueen (1986) found that for liquid iron, the product of density $\rho$ and $\gamma$ is 19.6(8) g/cm$^3$, which implies $\gamma = 1.59(9)$ at melting point of $\varepsilon$-Fe at 240 GPa. It is clear that there is some discrepancy in estimation of the Grüneisen parameter at condition of Earth core (Fig. 1). The present study determines the Grüneisen parameter for $\varepsilon$-iron on the basis of atom’s mean-square displacement from in situ high pressure and temperature X-ray investigations.

EXPERIMENTAL METHODS

Paskin (1957) suggested the dependence of Debye temperature $\theta$ on volume assuming that Grüneisen parameter is independent of volume:

$$\frac{\theta(V)}{\theta(V_0)} = \left( \frac{V_0}{V} \right)^\gamma$$

(2)

If $\gamma$ dependent on volume (see Eq. 1), the relationship between the Debye temperature and volume is given by Anderson (1995)

$$\ln \theta = \ln \theta_0 + \frac{\gamma_0}{q} \left[ 1 - \left( \frac{V}{V_0} \right)^\gamma \right].$$

(3)

<table>
<thead>
<tr>
<th>Phase</th>
<th>Pressure range, GPa</th>
<th>$\gamma_0$</th>
<th>$q$</th>
<th>Reference</th>
</tr>
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<tbody>
<tr>
<td>$\alpha$-iron</td>
<td>0–10</td>
<td>1.66</td>
<td>0.6</td>
<td>Boehler and Ramakrishnan (1980)</td>
</tr>
<tr>
<td>$\varepsilon$-iron</td>
<td>15–100</td>
<td>2.2</td>
<td>1.0</td>
<td>McQueen et al. (1970)</td>
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<tr>
<td>$\varepsilon$-iron</td>
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<td>2.2</td>
<td>1.62</td>
<td>Jeanloz (1979)</td>
</tr>
<tr>
<td>Liquid iron</td>
<td>243</td>
<td>1.59(9)</td>
<td></td>
<td>Brown and McQueen (1986)</td>
</tr>
<tr>
<td>$\varepsilon$-iron</td>
<td>0–240</td>
<td>1.7</td>
<td>0.7</td>
<td>Anderson (1998)</td>
</tr>
<tr>
<td>$\varepsilon$-iron</td>
<td>0–300</td>
<td>1.78(6)</td>
<td>0.69(10)</td>
<td>This work</td>
</tr>
</tbody>
</table>

* E-mail: Leonid.Dubrovinsky@geo.uu.se
† Current address: Center for Study of Matters at Extreme Conditions, Florida International University, PC 344, University Park, Miami, FL 33197; E-mail: saxenas@fiu.edu