Temperature distributions inside overdriven steady-plane shock wave fronts in iron

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Abstract

Temperature distributions inside overdriven steady-plane shock wave fronts in Fe for shocks up to 230 GPa are evaluated by applying temperature-dependent constant-volume specific heat to the equilibrium thermodynamic theory. Equilibrium thermodynamics can be applied to these shocks and the assumption of heat transport is valid. Thus, the inside temperature distributions are evaluated fairly correctly. Overestimations of the temperature distributions inside an inviscid solid Fe mean that the viscous pressure influences greatly on the distributions. The underestimation of the constant-volume specific heat in a higher pressure region causes the overestimation of the inside temperature distributions.

Keywords: Shock wave; Inside temperature distribution; Iron

1. Introduction

It is extremely important to know the physical properties of iron at high pressures because iron is considered principal element in the Earth’s core. The shock wave with a single structure above the pressure where the Hugoniot curve intersects with the Rayleigh line is called the overdriven shock wave. In this paper, temperature distributions inside the overdriven steady-plane shock wave fronts in iron in the regime of shock magnitude from 40 to 230 GPa are evaluated. The intersection point of the Hugoniot curve with the Rayleigh line is just below 40 GPa, and the melting occurs above 230 GPa.

The inside temperature (ITIM) method implicitly including heat transport was developed by Sano and Abe to estimate temperature distributions inside steady wave fronts in solids [1]. In this method, it is assumed that the state of the solid in the wave front is close to thermodynamic equilibrium, and that both heat transport and the work performed by thermal pressure in the wave fronts can be neglected because they could cancel each other out. The latter assumption of heat transport is valid if the viscous component of the pressure is large enough compared to the thermal component. Sano and Sano evaluated the temperature distributions in overdriven steady wave fronts shocked up to 80 GPa in 2024 Al, 250 GPa in Pt, and 230 GPa in Fe using the ITIM method [2]. The evaluated temperatures behind shock fronts using the ITIM method were sufficiently correct compared with the values calculated using Walsh–Christian theory [3]. The viscous components of the pressure were so large that the evaluated distributions were fairly correct. Therefore, two assumptions of thermodynamic equilibrium and heat transport were valid, and the ITIM method was effective.

Strain rates in overdriven steady-plane shock wave fronts induced by shocks up to 200–300 GPa might reach $10^{11}–10^{12}$ s$^{-1}$. The deformations at any material point inside the shock wave fronts do not change greatly during the electron–phonon relaxation time of 10–100 fs which is dominant up to 200–300 GPa. The homogeneous volumetric component of the deformation is even small because heterogeneous plastic flow on an atomic scale is very large. Consequently, the electron–phonon system can maintain itself near thermodynamic equilibrium for shocks up to 200–300 GPa, if the temporal rates of the change of inside temperatures are slower than the characteristic relaxation times of temperature. The homogeneous component supports a great part of the pressure on the Rayleigh line, which is used in thermodynamics of irreversible processes.
Therefore, irreversible thermodynamics can be applied to overdriven shocks up to 200–300 GPa, if strain rates are less than $10^{12}$ s$^{-1}$ and the states inside the shock wave fronts are regarded essentially as thermodynamic equilibrium.

It is known, however, whether irreversible thermodynamics is valid for overdriven shock waves because thermodynamic equilibrium of the states has not been determined. This question is still open because the macroscopic treatment of the material process is conceptually difficult without thermodynamics [4]. One method to answer this question is to verify that the system maintains itself near thermodynamic equilibrium. This can be verified by first calculating the process from irreversible thermodynamics and then comparing the characteristic times mentioned above with the temporal rates of change.

Sano and Sano calculated temperature distributions inside shock fronts in Fe for shocks up to 230 GPa using the temperature-independent constant-volume specific heat $C_V$ of Bass et al. [5] which is expressed by $C_V = 3Nk_B$, where $N$ is the number of atoms per unit mass and $k_B$ is the Boltzmann constant [2]. $C_V$ is, however, essentially temperature-dependent. Brown and McQueen represented the temperature-dependent equation of $C_V$ [6], and ab initio calculations supported this conception [7]. The main purpose of the present study is to calculate the physically valid change of temperatures through shock fronts, applying the temperature-dependent constant-volume specific heat to the ITIM method. The validity of the assumption of thermodynamic equilibrium is investigated for shocks in Fe up to 230 GPa which does not induce melting [6] by estimating the effective strain rates and temperature rise times. The validity of this method is investigated by comparing the viscous component of the pressure with the thermal component for this shock. In addition, temperature distributions inside overdriven steady wave fronts in inviscid Fe for a 230 GPa shock are evaluated using the equation for temperatures derived from Mie–Grüneisen equation, and the effect of the viscous pressure is investigated by comparing the value in an inviscid Fe with that in a viscous Fe. The inviscid solid means the solid, where viscous pressure is not induced during shock loading.

### 2. Equilibrium thermodynamic theory

First, the ITIM method is described. This method can treat adequately the temperature distributions inside shock fronts. Next, the method, which estimates the effective temperature thickness is presented. Finally, the equation which correctly estimates the temperature distributions in an inviscid solid is derived.

#### 2.1. Inside temperature method explicitly including heat transport

Sano and Abe developed the ITIM method, which estimates the temperature $T$ inside steady shock wave fronts in a solid [1]. Pressure $p$ inside the wave fronts is related to the specific volume $V$ by the Rayleigh line equation:

$$dp = -\rho U_0^2 dV,$$

where $U_0$ is the constant shock velocity, $\rho = 1/V$ is the material density, and subscript 0 refers to an ambient state. The following approximate equation is derived by assuming that heat transport and the work performed by thermal pressure could cancel each other out:

$$T dS = -(p - p_E) dV,$$

where $S$ is the entropy, and $p_E$ is the thermoelastic component of the pressure $p$. This assumption is valid if the work performed by the viscous pressure is sufficiently large compared with the work performed by the thermal pressure and heat transport. The set of equations used in this method consists of the irreversible thermodynamics obtained by equating Eq. (2) with the thermodynamic identity, the equation for cold pressure $p_C$, and the equation for thermoelastic pressure $p_E$. The thermodynamic equation is expressed by

$$C_V \frac{dT}{dV} + \gamma_0 \frac{V_0}{V} C_V T = -(p - p_E),$$

where $\gamma$ is the Grüneisen parameter, $C_V$ is the constant-volume specific heat on the Rayleigh line, and $\gamma/V = \gamma_0/V_0$ is assumed. The equation for cold pressure $p_C$ is given by

$$p_C = p_H - p_{r_H},$$

where $p_H$ is a known Hugoniot function which is represented as $p_H(V), p_{r_H}$ is the Hugoniot function $p_{r_H}(V)$ for thermal pressure, which is expressed by

$$p_{r_H} = \gamma_0 \frac{V_0}{V} \int_0^{T_H} C_V dT,$$

where $T_H$ is the temperature behind shock fronts, i.e. the Hugoniot temperature. The Hugoniot temperature $T_H$ is obtained using Walsh–Christian equation [3]:

$$C_{VH} \frac{dT_H}{dV_H} + C_{VH} \gamma_0 \frac{V_0}{V} T_H = \frac{1}{2} \frac{dp_H}{dV_H} (V_0 - V_H) + \frac{1}{2} (p_H - p_0).$$

The equation for $p_E$ is given by

$$p_E = p_C + p_T,$$

where $p_T$ is thermal pressure expressed by

$$p_T = \gamma_0 \frac{V_0}{V} \int_0^{T} C_V dT.$$
Brown and McQueen expressed constant-volume specific heat \( C_V \) in Fe as follows [6]:

\[
C_V = 3Nk_B + \Gamma T = 3Nk_B + \Gamma_0 \left( \frac{V}{V_0} \right)^{\frac{3}{2}} T,
\]

(9)

where \( \Gamma_0 = 0.091 \text{ J/kg K}^2 \) and \( g = 1.34 \).

Calculations are performed using the temperature-dependent constant-volume specific heat expressed by Eq. (9) in this study. Eqs. (3)–(8) are analyzed using a known Hugoniot function \( p_H(V) \) and a known Rayleigh line—pressure function \( p(V) \) to determine the temperature, cold pressure, thermoelastic pressure, and viscous pressure.

### 2.2. Effective temperature thickness

The effective thickness of the spatial profile of temperature (effective temperature thickness) is defined by Refs. [8–10]

\[
\frac{\Delta T}{\Delta Z} = \left| \frac{dT}{dZ} \right|_{\text{max}},
\]

(10)

where \( Z \) is the Lagrangian coordinate moving with the same velocity as the constant velocity of overdriven steady shock fronts, which is of an infinite width [11], and \( \Delta T = T_H - T_0 \). Therefore, it is assumed that the heat flux varies spatially slowly everywhere in the wave fronts. In general, the effective temperature thickness is greater than the effective specific volume thickness [8,9]. Derivative \( dT/dZ \) is related to the heat flux \( J(Z) \) by the steady heat conduction equation:

\[
J = -\frac{\kappa}{1 - \epsilon} \frac{dT}{dZ},
\]

(11)

where \( \kappa \) is the heat conductivity, and \( \epsilon(Z) = 1 - V(Z)/V_0 \) is the strain. Derivative \( dT/dZ \) has its maximum when \( (1 - \epsilon)J \) is maximum, and this yields

\[
\Delta Z = \frac{\kappa(T_H - T_0)}{[(1 - \epsilon)J]_{\text{max}}}.
\]

(12)

The continuity equation for heat transport is given by

\[
\frac{dJ}{dZ} = \rho_U s dQ \frac{dV}{dZ},
\]

(13)

where \( Q \) is the heat transferred to the material. The specific volume wave inside the steady wave front is assumed to expand from \( Z = 0 \) to \( \infty \). The following equation for the heat flux is obtained by integrating both sides of Eq. (13) from 0 to \( Z \) and using \( J(0) = J_H = 0 \)

\[
J = U_S(\epsilon_H - \epsilon) \frac{dQ}{dV},
\]

(14)

where \( \epsilon_H = 1 - V_H/V_0 \).

The quantity \( [(1 - \epsilon)J]_{\text{max}} \) in Eq. (12) is determined by incorporating Eq. (14) into the \( \Gamma T \) method. Here \( dQ/\frac{dV}{dV} = p_V - p_{S_0} \) is assumed, where \( p_{S_0} \) is the pressure which varies along an isentropic passing through the reference state. The effective temperature thickness is calculated, irrespective of the shape and the effective thickness of the specific volume wave.

### 2.3. Temperature in inviscid solids

The quadratic equation for the temperature \( T \) inside shock fronts is obtained by substituting the temperature-dependent constant-volume specific heat \( C_V \) expressed by Eq. (9) into Eq. (8). The solution of this equation is given by

\[
T = -\frac{3Nk_B + \sqrt{(3Nk_B)^2 + 2\Gamma p_0 V_0^2 p_T}}{\Gamma},
\]

(15)

where \( p_T = p - p_c \) for an inviscid solid. The pressure \( p \) is given correctly by Eq. (1) and the cold pressure \( p_c \) is evaluated correctly using Eqs. (4)–(6). Thus, Eq. (15) estimates the temperature distribution inside shock wave fronts in inviscid solids correctly. Eq. (15) is used to investigate the effect of the viscous pressure on the temperature distributions.

### 3. Results

#### 3.1. Thermodynamic equilibrium

We use the refined Hugoniot data of Brown et al. [12] as a known Hugoniot function \( p_H(V) \). The Hugoniot is shown in Fig. 1. The data used for calculation are listed in Table 1, where \( c \) and \( s \) are the constants expressed in the equation \( U_S = c + sU_p \), which is estimated from the solid region of the data of Brown et al. [12], where \( U_p \) is the particle velocity. \( C_V \) per \( Nk_B \) distribution obtained from calculations using these values is shown in Fig. 2 as a function of the Hugoniot pressure \( p_H \).

The effective temperature thicknesses \( \Delta Z \) and rise times \( \Delta \tau \) obtained using the \( \Gamma T \) method are listed in Table 2 for shocks up to 50, 100, 150, 200, 230 GPa, where

![Fig. 1. Hugoniot obtained using the linear \( U_S \) \( - \) \( U_p \) relation of Brown et al. [12].](image)
\( \Delta t \equiv \frac{\Delta Z}{U_S} \). In spite of the assumption that the heat flux varies gradually everywhere, the effective temperature thicknesses of the order of tens of nanometer indicate that there is a region where the temperature varies rapidly inside each shock front. In this region, heterogeneous plastic flow on an atomic scale is very large. The effective strain rates \( \dot{\varepsilon} \) calculated using the Hugoniot strain \( \varepsilon_H \) and \( \Delta t_S \equiv \Delta t/3 \) (see Refs. [8,9]) for shocks up to 50, 100, 150, 200, 230 GPa are also listed in Table 2. The effective strain rates of approximately \( 5.7 \times 10^{11} \, \text{s}^{-1} \) which includes relatively large plastic flow deformation component is obtained for 230 GPa shock. Even this strain rate yields the increment of the strain of only \( \sim 10^{-3} \) order during the electron–phonon relaxation time for metals (the order of 10 fs) which is dominant above the Debye temperature for shocks up to 200–300 GPa. In addition, the temperature rise time of approximately 1.8 ps for a 230 GPa shock is approximately 100 times longer compared with the relaxation time. Wallace discussed the equilibrium problem in solid metals in detail [13]. It is clear from Wallace’s discussion that the electron–phonon system remains near thermodynamic equilibrium even at the strain rate of the order of \( 10^{10} \, \text{s}^{-1} \). The range of the strain rates is from \( 0.7 \times 10^{11} \) to \( 5.7 \times 10^{11} \, \text{s}^{-1} \) for shocks from 50 to 230 GPa, and this range is larger than \( 10^{11} \, \text{s}^{-1} \). Thus, the assumption of thermodynamic equilibrium for shocks up to 230 GPa in Fe is valid.

### Table 1

| Input data for shock calculations in Fe [12,14] |
|-----------------------------------------------|
| Ambient temperature, \( T_0 \) (K) | 300 |
| Ambient density \( \rho_0 \) (g/cm\(^3\)) | 7.85 |
| \( c \) (km/s) | 3.855 |
| \( \dot{s} \) | 1.6196 |
| Grüneisen parameter, \( \gamma_0 \) | 1.69 |
| Thermal conductivity, \( \kappa \) (cal/cm s K) | 0.10 |

### Table 2

| Shock (GPa) | \( U_s \) (km/s) | \( \varepsilon_H \) | \( \Delta Z \) (nm) | \( \Delta t \) (ps) | \( \dot{\varepsilon} \) (10\(^{11}\) s\(^{-1}\)) |
|-------------|------------------|-----------------|-----------------|-----------------|------------------|
| 50          | 5.673            | 0.1979          | 47.26           | 8.331           | 0.713            |
| 100         | 6.862            | 0.2706          | 27.72           | 4.039           | 2.009            |
| 150         | 7.815            | 0.3129          | 21.61           | 2.765           | 3.394            |
| 200         | 8.634            | 0.3418          | 18.23           | 2.122           | 4.832            |
| 230         | 9.081            | 0.3553          | 16.94           | 1.865           | 5.716            |

#### 3.2. Validity of the ITIM method

Thermoelastic pressure distributions (dashed curves) obtained using the ITIM method for shocks of 50, 150, 200, and 230 GPa in Fe are shown in Fig. 3(a)–(d) together with the Rayleigh lines (heavy solid lines), the Hugoniots (solid curves), and the cold pressure distributions (dotted curves). It is verified in Ref. [1] that the assumption of heat transport is valid when the viscous pressure component \( P_v \) is sufficiently large compared with the thermal pressure component \( P_t = P_E - P_C \). Fig. 3(a)–(d) indicate the situation. Thus, the assumption of heat transport for shocks up to 230 GPa is valid. In addition, the validity of the fundamental assumption of thermodynamic equilibrium has been verified in the previous section. Therefore, the ITIM method is valid for shocks up to 230 GPa in Fe, that is, temperature distributions inside shock fronts (inside temperature distributions) are predicted to a good approximation.

#### 3.3. Influence of viscous pressure

The inside temperature distribution (dashed curve) calculated using the ITIM method and Eq. (15) for a 230 GPa shock in an inviscid Fe is shown in Fig. 4(a) together with the inside temperature distribution (heavy solid curve) in a viscous Fe and the temperature Hugoniot (solid curve) calculated using Eq. (6). This distribution is convex upward, because thermal pressure \( (P_T)_{IV} = p - p_C \) increases and then decreases with a decrease in specific volume, where subscript IV refers to an inviscid solid. It is much higher than that obtained using the ITIM method as shown in Fig. 4(a). The reason for this is accounted for using Eq. (15).

\( (P_T)_{IV} = p - p_C \) is obtained as mentioned above because \( p_E \equiv p \) for an inviscid solid. On the other hand, \( p_T = P_{EOS} - p_C \) is obtained for a solid which is not inviscid because \( P_E = P_{EOS} \), where \( P_{EOS} \) is a pressure on the equation-of-state surface. The thermal pressures differ because \( p \) is not equal to \( P_{EOS} \). It follows from \( (P_T)_{IV} > p_T \). Eq. (15) indicates that the temperature is high when the thermal pressure is large. Therefore, the high temperature for an inviscid Fe solid is due to the viscous pressure included in the temperature.
Calculation. Fig. 3(a)–(d) indicates that the viscous pressure component is sufficiently large for any shock, and that the viscous pressure component increases with shock loading. As a result, the difference of the temperature distributions between an inviscid and a viscous solids increases with shock loading.

The temperature Hugoniot (solid curve), the inside temperature distributions for a viscous (heavy solid curve) and an inviscid (dashed curve) Fe solids calculated using temperature-independent $C_V = \frac{3Nk}{B}$ for a 230 GPa shock are shown in Fig. 4(b). These distributions are higher than those calculated using temperature-dependent $C_V$ as shown in Fig. 4(a). These overestimation of temperature distributions calculated using temperature-independent $C_V$ is due to the underestimation of $C_V$ as shown in Fig. 2.

4. Conclusions

Temperature distributions inside overdriven steady-plane wave fronts in solid Fe shocked up to 230 GPa, where melting does not occur, were evaluated by applying the temperature-dependent constant-volume specific heat to the inside temperature method implicitly including heat transport which is based on the equilibrium thermodynamic theory. The inside temperature distributions are evaluated fairly correctly because a fundamental assumption that the solid state inside the wave fronts is close to the thermodynamic equilibrium and another assumption on heat transport are valid. Overestimations of inside temperature distributions in an inviscid solid Fe indicate that the viscous
pressure influences the distributions. The underestimation of constant-volume specific heat in a higher pressure region causes the overestimation of the temperature distributions.

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