Equation of state for indium in shock waves

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Abstract. A model of the equation of state in the form of pressure as a function of density
and specific internal energy is used to describe the properties of indium. Thermodynamic
characteristics of this metal at high pressures are calculated and compared with the available
experimental data on shock compressibility.

1. Introduction
Numerical simulations of physical processes at high energy densities demand equations of state
for materials in question [1–3]. In processes those related with influences of intense laser [4–6]
and particle beams [7,8] upon condensed matter, impacts of high velocity bodies [9,10], electrical
explosions of conductors by powerful current pulses [11–15], states of materials can be realized
in a wide range of thermodynamic parameters. Modeling of the equation of state over such
a range is possible in the framework of the semiempirical approach [1], in which a functional
relationship between thermodynamic parameters is chosen from theoretical considerations, as
well as numerical coefficients in this relationship are determined with the use of experimental
data.

Indium has a high neutron-capture cross-section for thermal neutrons; therefore, it is used as
a material of control rods in nuclear reactors. Equation of state (EOS) for indium is of particular
interest for simulations of some processes in such reactors.

In this work, the caloric model $P(V,E)$ [16–19] is used to thermodynamically describe the
properties of indium under shock compression. Here, $P$ is the pressure, $V$ is the specific volume,
$V = \rho^{-1}$, $\rho$ is the density, $E$ is the specific internal energy. The EOS has been obtained and
used for calculations of the principal Hugoniot adiabat, which is compared with the available
data of shock-wave measurements at high pressures [20–23].

2. EOS model
The EOS model is chosen based on the quasiharmonic approximation with taking into account
anharmonic effects [24]. The model has a general form

$$P(V,E) = P_c(V) + \frac{\Gamma(V,E)}{V} [E - E_c(V)], \quad (1)$$

where $E_c$ is a cold component of the energy at zero temperature $T = 0$; $P_c = -dE_c/dV$ is the
corresponding cold pressure at $T = 0$; $\Gamma$ is a coefficient determining thermal contributions to
the EOS.
The volume-dependent cold energy is taken as a polynomial \[25, 26\]

\[
E_c(V) = \frac{B_{0c}V_{0c}}{m-n} \left( \frac{\sigma_m}{m} - \frac{\sigma_n}{n} \right) + E_{\text{sub}},
\]

where \(\sigma_c = V_{0c}/V\); \(V_{0c}\) and \(B_{0c}\) are the specific volume and bulk modulus at \(P = 0\) and \(T = 0\); \(E_{\text{sub}}\) has meaning of the sublimation energy. The latter is determined by a normalizing condition

\[
E_c(V_{0c}) = 0,
\]

from which one can obtain

\[
E_{\text{sub}} = \frac{B_{0c}V_{0c}}{mn}.
\]

The coefficient \(\Gamma\) \[27–29\] depends on both the volume and the energy as

\[
\Gamma(V, E) = \gamma_i + \gamma_c(V) - \gamma_i \frac{1 + \sigma_{c}^{-2/3} (E - E_c(V))}{E_n}.
\]

Here, \(\sigma = V_0/V\); \(V_0\) is the specific volume under normal conditions \(P = 0\), \(E = E_0\). At low thermal energies \(E - E_c \ll E_0\sigma^{2/3}\), \(\Gamma \approx \gamma_c(V)\); in the opposite case \(E - E_c \gg E_0\sigma^{2/3}\), \(\Gamma\) becomes equal to the constant \(\gamma_i\). The energy \(E_a\) is determined from results of experiments with strong shock waves. The function of \(\gamma_c\) upon \(V\) is taken as

\[
\gamma_c(V) = 2/3 + (\gamma_{0c} - 2/3) \frac{\sigma_n^2 + \ln^2 \sigma_m}{\sigma_n^2 + \ln^2 (\sigma/\sigma_m)},
\]

where the parameters \(\sigma_n\) and \(\sigma_m\) are generally found from the condition of optimum description of shock-wave data, and

\[
\gamma_{0c} = \gamma_i + (\gamma_0 - \gamma_i) \left[ 1 + \frac{E_0 - E_c(V_0)}{E_n} \right]^2,
\]

\(\gamma_0\) is the Grüneisen coefficient \(\gamma = V(\partial P/\partial E)/V\) under normal conditions, \(\gamma(V_0, E_0) = \gamma_0\).

3. EOS for indium

Indium under atmospheric pressure has a body-centered tetragonal (bct) structure \[30–34\], which can be also represented as a face-centered tetragonal (fct) one. It melts at 430 K \[30\]. Under compression at room temperature, the fct phase transforms to a face-centered orthorhombic (fco) structure at about 45 GPa without evident change of volume \[31, 32\]. At further increase of pressure, more phase transformations of indium were predicted using methods of electron structure calculation \[35–37\]. In recent experiments \[34\], a transition of the fco phase to the fct one is determined at compression up to about 150 GPa.

Shock compressibility of indium is studied with the use of traditional explosive systems up to about 150 GPa \[20–23\] and with special explosive systems up to 350 GPa \[23\]. The data of shock-wave experiments \[20–23\] can be generalized as a linear relationship between the velocities of the shock front \((U_s)\) and the particles behind the front \((U_p)\),

\[
U_s = a + bU_p,
\]

where \(a = 2.56 \text{ km/s}\), and \(b = 1.477\) \[38\]. One can calculate specific volume and pressure along the Hugoniot adiabat using the conservation laws \[1\] for mass,

\[
V = V_00 \frac{U_s - U_p}{U_s},
\]

and momentum,

\[
P = P_0 + \frac{U_sU_p}{V_00},
\]
Figure 1. The Hugoniot adiabat (H), the room-temperature isotherm and the cold curve ($P_c$) of indium: solid lines—adiabats (black—calculated with the present EOS; green—EOS [39]; red—relations (8)–(10) with parameters from compendium [38]); black dash-dot line—isotherm $T = 0$ from the present EOS; green dash-dot line—isotherm $T = 298$ K [39]; markers—experimental data on static compression at room temperature (T1—fct [31]; T3—fct [33]; T4 and T5—fct and fco respectively [34], where pressure is recalculated with EOS of Pt standard [40]) and shock loading (H1—[20]; H2—[21]; H3—[22]; H4—[23]).

where $V_0$ and $P_0$ are the initial specific volume and the initial pressure before the shock front.

In this work, EOS for the fct-solid and liquid phases of indium is constructed. The EOS coefficients for In are as follows: $V_0 = 0.1372$ cm$^3$/g, $V_{0c} = 0.13431$ cm$^3$/g, $B_{0c} = 45.68768$ GPa, $m = 1.42$, $n = 1.43$, $\sigma_m = 0.85$, $\sigma_n = 0.81$, $\gamma_{0c} = 2.31$, $\gamma_1 = 0.45$ and $E_a = 90$ kJ/g.

Calculated cold curve and principal Hugoniot adiabat of indium are shown in figure 1 along with data on both static compression at room temperature [31,33,34] and shock loading [20–23] up to 80 GPa. Also, the EOS results in figure 1 are compared with room-temperature isotherm and shock adiabat calculated with the use of EOS for this metal [39] as well as with shock adiabat based on relation (8) with parameters from compendium [38]. In the cases of the two EOSs, which both have a form $P(V, E)$, the conservation law [1] for energy,

$$E = E_0 + \frac{1}{2}(P + P_0)(V_00 - V),$$

was used to calculate pressure and density of shock-loaded matter. Here, $E_0$ is the initial specific internal energy before the shock front; $P_0 = 0.1$ MPa; $V_{00} = V_0$ according to the EOS. In the case of relation (8), equations (9) and (10) were used with $V_{00} = V_0^{-1}$, $\rho_0 = 7.3$ g/cm$^3$ [38].

As can be seen in figure 1, the present EOS is consistent with data from both static and dynamic measurements. The Hugoniot adiabat calculated using EOS [39] lies at somewhat higher densities when compared with the data [20–23].

Same calculation results are shown along with experimental data [20–23, 31–34] in whole investigated range of shock and particle velocities, pressures and densities in figures 2 and 3. It
can be seen that the EOS [39] significantly underestimates the shock velocity at a given particle velocity, as well as the shock-wave pressure at a given density.
4. Conclusion

EOS in the form of an analytic function is proposed for indium in the fct-solid and liquid phases. This EOS agrees well with available data from experiments with shock waves. One can use the EOS effectively in numerical simulations of physical processes in the metal at high pressures.

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