# Simulation of generation of high pressure and temperature in metals under shock loading

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**Abstract.** *Pressure and Temperature in different metals including radioactive materials behind converging shock waves, is simulated using generalized form of equation of state. Tait's equation of state of metals, is valid for pressures of the range of few mega bars and takes into account only elastic pressures. At such high pressures, metal undergo phase change and normal equation of state no more is valid. At such pressures, temperatures in metals becomes very high and thermal and excitation pressures dominate over elastic pressure. It is observed that as shock approaches the center of sphere, excitation pressure dominates elastic as well as thermal pressure.*

**Key words.** Phase change, shocks in metals and radioactive materials.

## 1. Introduction

Simulation of high pressure and temperature generated by imploding shock waves through condensed media, such as metals and radioactive materials, is of great theoretical and practical importance. Behavior of metals under high pressures has been analyzed by many authors [1-4], by taking into account, the general Hugoniot relationship between shock velocity and particle velocity. This linear equation fails when we analyze the material undergoing crystallographic phase change under high pressure. Thus, knowledge of the thermodynamic properties of the materials is necessary to study their behavior under high pressures and temperatures. Although, no appreciable [2] difficulties are encountered in calculating the thermodynamic properties of gases, a theoretical description of the thermodynamic properties of solids and liquids at high pressure generated by very strong shocks, present a very complex problem.

Variation of material parameters under shock loading has been studied by Singh and Renuka [5], by taking thermodynamic properties of the materials into account. In this paper, total energy of system is taken as sum of cold, excitation and thermal energy. By taking thermal energy as $C_V T$ ,with $C_V$ constant, it was shown that discontinuities in pressure can be removed at ultra high pressure. In this process, a very strong compression of a condensed medium generates a colossal internal pressure, even in the absence of heating due only to the repulsive forces between the atoms. The material is also very strongly heated by shock waves and, this results in the appearance of a pressure associated with the thermal motion of atoms. It is known that thermal energy is not linear function of temperature and $C_V$ also varies with temperature. In the present paper we have taken Einstein Equation for thermal energy and have studied the pressure and temperature variations behind the converging shock waves. Results of variation of pressure by conventional method and by present method are compared in table-3.

## 2. Formulation of the Problem

It is assumed that a spherical shock wave is moving from the surface of a metal (or radioactive material) sphere towards its center. Generalised thermal l energy of materials given by Einstein Equation of state ,

$$E_T = 3N \frac{h\nu}{[\exp(h\nu / kT) - 1]} \quad (1)$$

Is used along with jump conditions [2] to get expressions for pressure and temperature behind imploding shock waves. In equation (1) N, h, $\nu$, k are Avagadro's Number, Plank's constant, natural frequency of solid material, and Boltzman's constant respectively.

Excitation energy of metals is given by[2,5]

$$E_e = \frac{1}{2} \beta_o \left( \frac{\rho_0}{\rho} \right)^{1/2} T^2 \quad and \quad \beta_o = 21.179 \frac{k^2 m_e}{h^2} N_e^{1/3} \left( \frac{1}{\rho_1} \right)^{2/3} \quad (2a)$$

where $m_e$ is the electron mass, and $N_e$ is the number of free electrons per unit volume of the metal.

Cold energy is given by,

$$E_c = -\int P_c dV \quad (2b)$$

Equations for cold, thermal and excitation pressure are,

$$P_c = A(S) \left[ \left( \frac{\rho}{\rho_0} \right)^n - 1 \right] \quad (3a)$$

$$P_T = \Gamma(V) \frac{E_T}{V} \quad (3b)$$

$$P_e = \frac{1}{2} \frac{E_e}{V} \quad (3c)$$

where V is specific volume and [5],

$$\Gamma(V) = -\frac{2}{3} - \frac{V}{2} \frac{(d^2 Pc / dV^2)}{(dPc / dV)} \quad (3d)$$

Using equations(1)-(3), total pressure P and energy E behind the shock front is obtained,

$$P = A(\delta^n - 1) + \frac{3N\Gamma\rho_0\delta\, k\,\Theta}{(e^{\Theta/T} - 1)} + \frac{1}{4}\rho_0\beta_0\delta^{1/2}T^2 \tag{4a}$$

$$E = \frac{A}{\rho_0}\left[\frac{(\delta^n + n - 1)}{\delta(n-1)}\right] + \frac{3Nk\,\Theta}{(e^{\Theta/T} - 1)} + \frac{1}{4}\beta_0\delta^{-1/2}T^2 \tag{4b}$$

Here $\Theta = h\nu/k,$ is Debye's constant and $\delta = \frac{\rho}{\rho_0} = Shock\,strength.$ We observe from relations (4) that pressure P is function of density ratio $\delta$ and temperature T. We take $\delta$ as the independent parameter and express all other paraameters in terms of $\delta$. Elliminating U and u from equations (1) of [2], one gets,

$$(\delta - 1)(P + 2P_0) = 2\rho_0\delta E \tag{5}$$

where $P=P_2-P_0$ and $E=E_2-E_0$.

Differentiating this equation with respect to $\delta$, we get,

$$(P + 2P_0) + (\delta - 1)\frac{dP}{d\delta} = 2\rho_0 E + 2\rho_0\delta\frac{dE}{d\delta} \tag{6}$$

Using equations (4) in (5) and after some algebraic calculations, we get,

$$\frac{dT}{d\delta} = \frac{f(T,\delta)}{g(T,\delta)} \tag{7}$$

where

$$f(T,\delta) = -\rho_1\left[\frac{A}{\rho_1\delta}\left\{n\delta^{n+1} - (n+2)\delta^n + 2\right\} + \frac{T^2\beta_0}{8\sqrt{\delta}}\left\{\delta + 3\right\} - 2\,\rho_1\,E + P_2(T,\delta)/\rho_0 + P_0/\rho_0\right]$$

$$g(T,\delta) = \left[\frac{3N\Gamma_0\rho_0 k\,x^2(\delta - 1)}{(e^x - 1)^2} + \frac{\rho_0\beta_0 T(\delta - 5)\sqrt{\delta}}{2} + \frac{6Nk\Theta^2\rho_0\delta}{T^2(e^x - 1)^2}\right] \tag{8}$$

$$x = \frac{h\nu}{kT},\ \Gamma = \Gamma_0/\delta \quad (ref[6])$$

We get T in terms of $\delta$, from this equation, and then using equation (4) for P, other parameters can be computed from,

$$\mathrm{U} = \sqrt{\frac{\mathrm{P}\delta}{\rho_1(\delta - 1)}} \tag{9}$$

$$\mathrm{u}_2 = \sqrt{\frac{\mathrm{P}(\delta - 1)}{\rho_1\,\delta}} \tag{10}$$

In the above equations, natural frequency of the metal is slightly complex parameter. This is computed by replacing it by Debye's temperature given by,

$$\Theta = h\nu / k \tag{11}$$

Values of Debye's temperature for different metals is given in table -2, and basic parameters are given in table-1.

## 3. Solution of the problem

The equations (1) to (4) are solved to get the pressure, temperature, shock velocity and particle velocity of the material behind the shock front. These parameters are expressed in terms of $\delta$ and T. It is not possible to solve these equations explicitly in terms of one parameter, say $\delta$. Therefore temperature is expressed in differential form and evaluated by integrating equation (7) using Runge –Kutta method of fourth order.

In order to express pressure and temperature in terms of the distance 'r' of the shock front from the center of the sphere, we use Energy Hypothesis [6]. Transmitted pressure due to the initial compression of the metal by the shock transmitted from explosive to material at its outer boundary is calculated using mismatch conditions [6].

Variation of $\delta$ as the shock moves from the surface of metallic sphere to its apex is calculated by using energy hypothesis [6] as,

$$\left(\frac{r_o}{r}\right)^3 = \frac{\delta}{\delta_i}\frac{\overline{E}(\delta)}{\overline{E}(\delta_i)} \tag{12}$$

where index 'i' denotes, values at the explosive- material boundary. Energy $\overline{E}(\delta)$ is given by

$$\overline{E}(\delta) = E(\delta) + \frac{1}{2}u_2^2 \tag{13}$$

where $E(\delta)$ is given by equation (4b).

Knowing $\delta$ as a function of $r/r_0$, other parameters are evaluated from equations (2)-(4).

## 4 Results and Discussion

In this paper, we have considered five materials, of which two are radioactive in nature (Table 1).

Variation of pressure for Al, Fe, Stainless Steel (Type 404), Molybdenum (Mo), and Iridium is shown in Figure 1, where as variation of temperature for these metals is given in figures 2. Transmitted pressure in Aluminum is low at the metal-explosive interface but rises fast and becomes infinite at radius equal to 0.3. Similarly pressure in Iron grows faster than Stainless steel. In Molybdenum (Mo), pressure rise is slow as compared to lighter metals, and becomes infinite at radius ratio 0.1. In figure -3, we have plotted variation of cold, thermal and elastic pressures in Iron. It is seen that in the beginning thermal and elastic pressures are less than cold pressure but ultimately, thermal pressure and excitation pressure increase and become more than elastic pressure. Excitation pressure increases very fast and becomes maximum at radius 0.3 and then starts reducing.

It has been observed that as the density of material increases, its maximum compression as well as transmitted pressure from explosive decrease (Table-2).

## Conclusion

In studying the pressure variation across the shock using Hugoniot equation of state, it has been observed that at high pressures, certain materials show sudden increase in pressure values or even a discontinuity in the pressure curve as the shock wave converges from the surface of the sphere to its center [5]. This is because this equation does not take into account the thermal and excitation energy of metals. Figure-3 gives three pressure components for a typical metal, say Iron. It shows that, $P_T$ and $P_e$ are of same order initially, but ultimately $P_e$ becomes much more that $P_T$ . Near the centre, effect of excitation pressure is to expand where as it is resisted by elastic pressure, which creates a uncertainty at such points, resulting in the abnormal behavior of $P_e$ curve. Thermal pressure first increases and then becomes almost constant and when shock approaches near the centre, again rises. Figure-1 gives pressure variations, where as figure- 2 gives variation of temperature as shock converges.

## Acknowledgement

Present work was funded by Defence Research and Development,, Ministry of Defence.

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## Table 1 Data used in this paper

| Material | A Bars | $\Gamma_O$ | $\Gamma$ at boundary | n | $\beta$ erg/g.deg$^2$ | $\rho$ g/cm$^3$ | $E_0$ $10^8$ erg/g |
|---|---|---|---|---|---|---|---|
| Al | 1.8200 e+010 | 2.0 | 1.35 | 4.352 | 500 | 2.785 | 16.1 |
| SS | 3.3233 e+010 | 2.17 | 1.49 | 4.96 | 540.6 | 7.896 | 12.9 |
| Fe | 1.5010 e+010 | 1.69 | 1.56 | 6.68 | 541 | 7.85 | 12.85 |
| Mo | 6.8150 e+010 | 1.520 | 1.39 | 3.932 | 495 | 10.206 | 7.2 |

**Table 2. Comparison table showing pressure values at few points**

| Sr. No | Metal | Debey's Temperature $\Theta\,^{o}K$ | $\delta$ | $\delta_i$ | $\delta_{max}$ |
|---|---|---|---|---|---|
| 1. | Aluminum | 428 | 2785 | 1.25213 | 1.31154 |
| 2. | Iron | 470 | 7850 | 1.2146 | 1.2437 |
| 3. | Stainless Steel | 470 | 7896 | 1.1689 | 1.1899 |
| 4. | Molybdenum | 450 | 10206 | 1.09422 | 1.1035 |
| 5. | Iridium | 420 | 10484 | 1.08848 | 1.1035 |

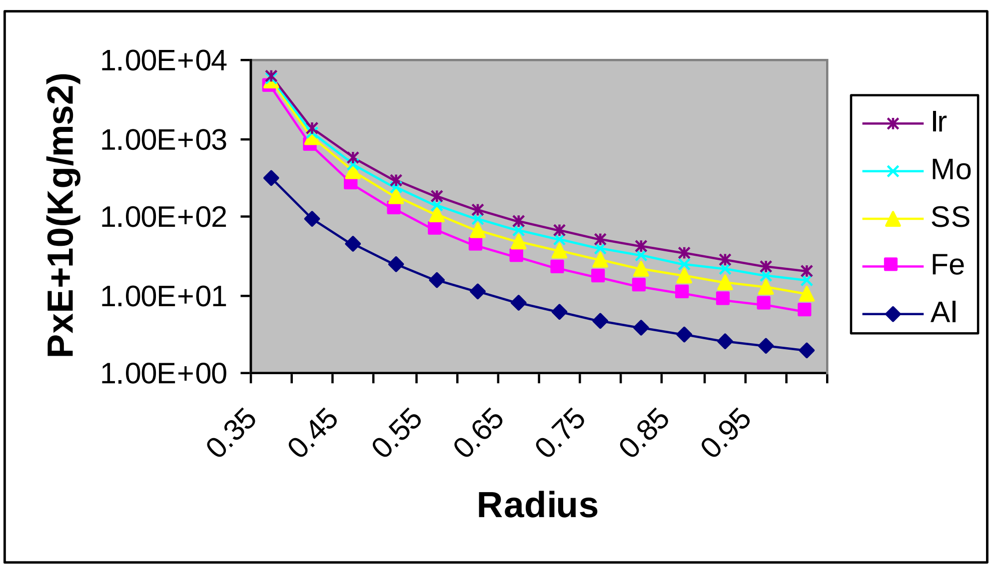


**Figure-1: Variation of pressure Vs dimensionless radius for different materials**

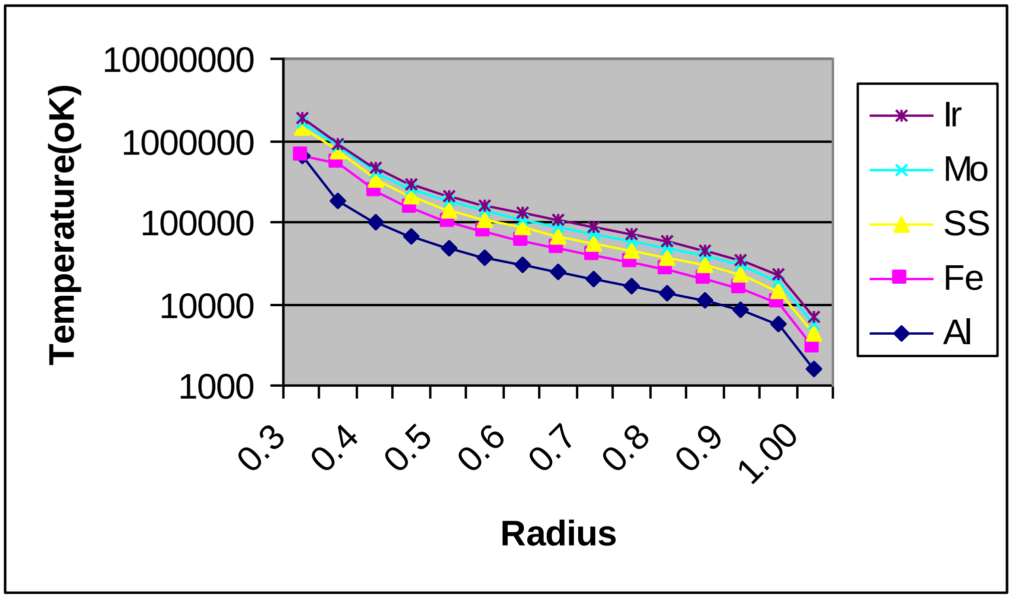


**Figure-2: Variation of temperature Vs dimensionless radius for different materials**

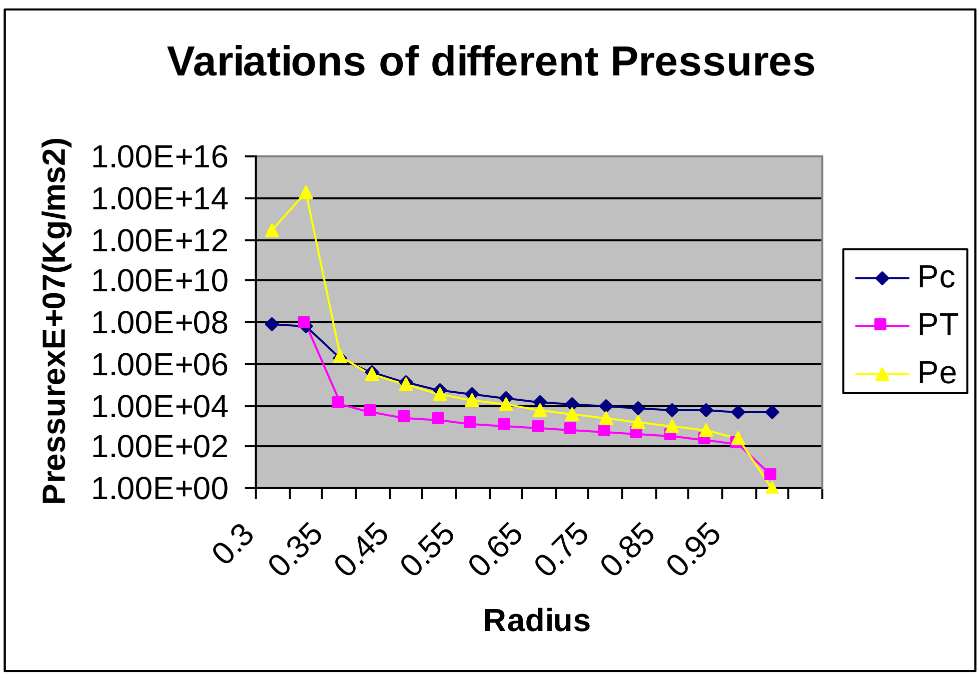


**Figure 3: Comparison of three components of pressure**