# Numerical analysis of explosively generated shocks in a Ti-Al powder mixture

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Three constitutive models have been applied to computationally model explosively generated shock waves in a 304 stainless steel recovery capsule containing a Ti-Al powder mixture. The models used are the classical Mie-Gruneisen model, the VI model (Void-Inert) proposed herein and the VIR model (Void-Inert-Reactive) previously proposed by Bennett and Horie. The formation of weak Mach reflections in the powder mixture due to the difference between the explosive detonation velocity and the shock wave velocity in the powder mixture is observed. Large differences are observed in the computed temperature profiles between the Mie-Gruneisen and VI (or VIR) models. The residual temperature profiles may be significant to the reacted regions observed in the actual experiments.

## 1. Introduction

Shock-induced reactions in intermetallic and metallic-ceramic powder mixtures offer one method to synthesize novel compounds at high pressures[1]. These reactions may benefit from the partial or full collapse of the pores between the powder particles by the shock wave. The distribution of the pore collapse energy may favor the more ductile constituents and be centered around the pore collapse points to produce short lived but extreme hot-spots within the compressed mixture[2]. These hot-spots will rapidly equilibrate with the surrounding "cold" material due to thermal conduction and mass transport, but they could serve as reaction initiation points. Previous investigations have indicated that significant if not complete "shock-induced reactions" can take place at a 100 ns rate during and just behind the shock front in the powder mixture[3-5] as opposed to "shock assisted reactions" which may benefit from the shock wave environment, but occur after the shock pressure is released[6].

For the explosive loading experiment modeled here, a 1:1 atomic ratio mixture of spherical Ti and Al powder was initially compressed to an initial porosity of 20% in a double walled 304 stainless steel (304 SS) recovery capsule with screw on caps[7], as seen in Figure 1. The capsule was surrounded with nitromethane or commercial emulsion explosive in a plastic tube and topped with an explosive lens that produced a planar detonation around the capsule[8]. The detonation speed in the explosive is greater than the shock speed in the capsule and powder mixture, so a weak Mach reflection develops along the center axis of the powder mixture. Within this Mach reflection the shock pressure and temperature as well as the residual temperature will be significantly higher than that outside of it. A zone of higher particle velocity than the surrounding powder called a slip stream is formed behind the Mach reflection which could be a source of additional mass mixing.

The recovered specimens form these experiments were cut open axially and polished for material analysis. A region of fully reacted material was observed in the center of the specimens roughly corresponding to the slip stream region. The surroun-

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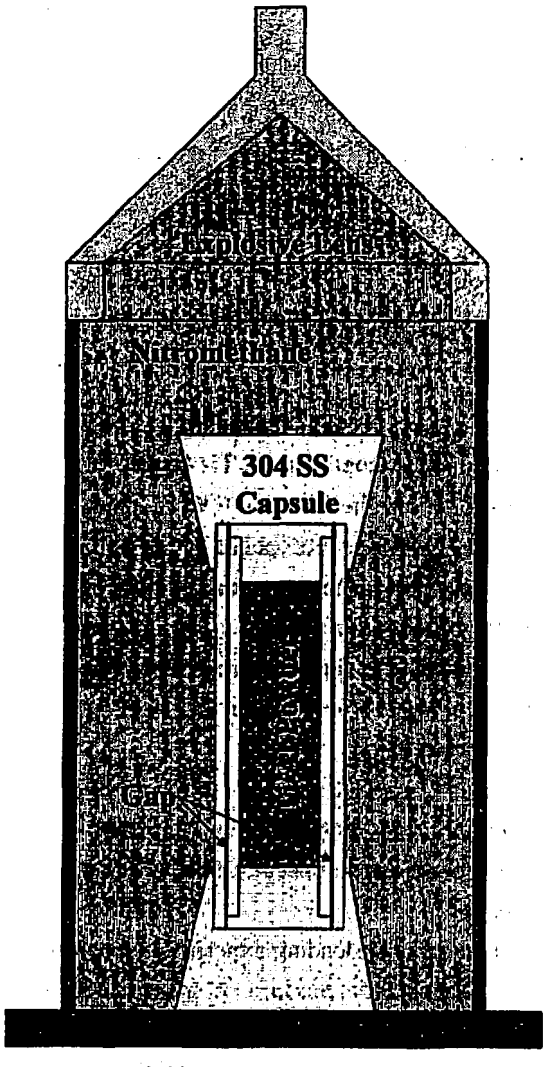


Fig. 1 The experimental arrangement for explosive loading and recovery

ding material was fully compressed but not reacted Ti and Al particles. It is unclear from these recovered specimens whether the reaction took place during the shock wave or afterwards due to the high residual temperatures. In this study, the experiments were computationally modeled using three constitutive models implemented on two different numerical hydrocodes to correlate the Mach reflection pressure and temperature profiles to the reacted regions observed.

## 2. Computation

Multiple constitutive models of powder material response to shock compression exist. The simpler models treat the powder mixture as an inert continuum which responds as a bulk material, while more complex models separate the individual constituents of the powder mixture, account for chemical reactions between the constituents, and include the formation of hot-spots and subsequent heat transfer to the surrounding "cold" constituents.

This paper will compare the results of three of these models as they are employed to model the Ti-Al powder mixture experiments.

### 2.1 2－DL Model

The first model used to model this experiment is the two dimensional Lagrangian hydrocode 2－DL[8]. This model employs the classical constitutive modeling approach of only altering the equation of state (EOS) used to describe the inert powder mixture and leaves the hydrodynamic conservation of mass, momentum, and energy equations in their original forms. The Mie-Grüeisen relation, $P-P_R=(\Gamma/v)(E-E_R)$, is applied to account for the additional energy deposited into the inert solid as the pores collapse where P is the shock pressure, v is the specific volume, E is the specific internal energy, $\Gamma$ is the Grüeisen parameter defined $\Gamma=v(\partial P/\partial E)_v$, and the subscript R refers to a reference state. The reference state is taken as the ideal shock Hugoniot of a solid material whose shock properties are calculated from those of the individual constituents by mass fraction mixing.

In this case, an EOS based on the linear shock velocity-particle velocity ($U_s-u_p$) relation, $U_s=C_0+Su_p$, is employed to describe the reference $P_R-v_R$ Hugoniot,

$$P_R-P_o=\frac{C_o^2(1-v_R/v_{oo})}{v_{oo}[1-S(1-v_R/v_{oo})]^2} \qquad (1)$$

where $C_o$ is the initial bulk sound speed, S is the $U_s-u_p$ slope, and $v_{oo}=1/\rho_{oo}$ is the initial specific volume of the solid mixture. Thus, the shock pressure is a function of specific volume and internal energy, P(v,E). The temperature is calculated as only a function of the internal energy, $T=T_R+(E-E_R)/C_v$, where $C_v$ is the constant volume specific heat.

The pore collapse is modeled by an exponential $P-\alpha$ equation which essentially fits a curve between the initial zero pressure specific volume of the mixture, $v_{oo}$, and the above described EOS used to describe the powder mixture,

$$\alpha=1+(\alpha_o-1)\exp\left[-\frac{P}{P_T^*}\right] \qquad (2)$$

In eq.(2), the distention ratio is defined as $\alpha=v/v_s$

Table 1 Properties used in these calculations

| | $Al_{(s)}$ | $Ti_{(s)}$ | $Ti_{(s)}:Al_{(s)}$ | 304 SS |
|---|---|---|---|---|
| $\rho_{os}$(kg/m³) | 2707 | 4530 | 3645 | 7900 |
| $\lambda_i$ | 0.3604 | 0.6396 | 1.0 | |
| $C_o$(m/s) | 5386 | 5020 | 5003 | 4570 |
| S | 1.34 | 0.98 | 1.24 | 1.49 |
| $\beta_{To}$(GPa) | 76.7 | 107.7 | 91.3 | 165.0 |
| $\beta_{To}'$ | 4.36 | 2.92 | 3.96 | 4.96 |
| $\Gamma$ | 2.0 | 1.09 | 1.42 | 2.2 |
| $C_v$(kJ/kgK) | 0.884 | 0.705 | 0.770 | 0.440 |

| $P=A\left(1-\frac{\omega\rho}{R_1\rho_{ref}}\right)exp\left[\frac{-R_1\rho_{ref}}{\rho}\right]+B\left(1-\frac{\omega\rho}{R_2\rho_{ref}}\right)exp\left[\frac{-R_2\rho_{ref}}{\rho}\right]+\omega\rho e_s$ (JWL) | Nitromethane |
|---|---|
| Reference density, $\rho_{ref}$ (g/cm³) | 1.128 |
| Parameter A (Mbar) | 2.0925 |
| Parameter B (Mbar) | 0.05689 |
| Parameter $R_1$ | 4.4 |
| Parameter $R_2$ | 1.2 |
| Parameter $\omega$ | 0.3 |
| Detonation velocity, D (cm/$\mu$s) | 0.628 |
| Energy/unit volume, $e_s$ (Mbar) | 0.051 |

where $v_s$ is the specific volume on the compressed powder EOS, $\alpha_o$ is its initial zero pressure value, and $P_T^*$ is a pressure constant controlling the pore collapse.

For this case, the nitromethane, capsule, and powder were all modeled in Lagrangian coordinates and the double walled capsule was modeled as one thick wall. The material properties used for the KHT model[9] describing the nitromethane detonation, $U_s-u_p$ equations[10] of the 304 SS and the Ti-Al mixture are given in Table 1. In this model the Grüeisen parameter was assumed to remain constant, $\Gamma=\Gamma_o$, throughout the computation. Pressure and temperature contour plots in the Ti-Al mixture by this model with $P_T^*=1.864$ GPa, i.e. a crush-up pressure of 6.0 GPa, are displayed in Figure 2. The weak Mach reflection is evident in the pressure contours. The residual temperatures do not seem related to the reaction regions observed in the recovered specimen[7].

A parametric study of the pore collapse pressure was performed to investigate its effects on the Mach reflection. The Mach stem width was shown to increase with decreases in the pore collapse pressure.

### 2.2 VI and VIR Models

The second and third models both employ a constitutive method that simultaneously solves the hydrodynamic conservation of energy equation in Lagrangian coordinates,

$$dE_s=-(P+\eta)dv \qquad (3)$$

and an EOS where $\eta$ is the artificial viscosity. For both of the calculations given here, the Birch-Murnaghan EOS is used to describe the response of the

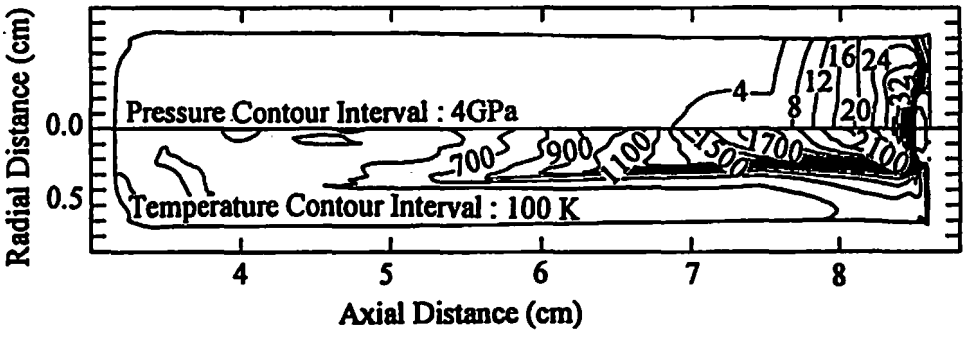


Fig. 2 Pressure and temperature contour plots at 16.0 $\mu$sec as calculated by the 2 − DL hydrocode for a low pore collapse pressure

solid material (x) as a pressure, specific volume, and temperature function,

$$P_x(v_x,T_x)=\frac{\beta_{T\alpha x}}{\beta'_{T\alpha x}}\left[\left(\frac{V_x}{V_{x\alpha}}\right)^{\beta'_{T\alpha x}}-1\right]+\left[\frac{\Gamma_x}{V_{x0}}\right]C_{vx}(T_x-T_0) \quad (4)$$

where $\beta_{T\alpha x}$ is the isothermal bulk modulus, and $\beta_{T\alpha x}$ is its first pressure derivative. In this EOS, the Gruneisen ratio is assumed to remain constant, $\Gamma/v=(\Gamma/v)_o$, throughout the computation. These equations are linked through the second law of thermodynamics for either an inert system,

$$dE_x=T_x ds_x-P_x dv_x \quad (5)$$

as in the VI model, or for a reactive system,

$$dE_x=T_x ds_x-P_x dv_x+\sum_{j=1}^{n}\lambda_{xj}\,g_{xj} \quad (6)$$

as in the VIR model[2]. In eq.(6), $\lambda_{xj}$ is the mass fraction of constituent j in solid x and $g_{xj}$ is its Gibb's free energy.

### 2.2.1 VI Model

In the case of an inert system, a new model has been developed using the same idealized solid mixture assumption as in the 2 − DL model. The powder may be described in terms of an idealized solid whose properties are determined from those of the individual constituents through mass fraction based mixing. From Ref. 4, the mean specific volume is described $v_{xj}=\sum_{j=1}^{n}\lambda_{xj}v_{xj}$, the mean specific heat is $C_{xj}=\sum_{j=1}^{n}\lambda_{xj}C_{xj}$, the mean Grüeisen parameter is $\Gamma_{xj}=\sum_{j=1}^{n}\lambda_{xj}\Gamma_{xj}$, the mean isothermal bulk modulus is

$$\beta_{T\alpha x}=\frac{V_x}{\sum_{j=1}^{n}\frac{\lambda_{xj}v_{xj}}{\beta_{T\alpha x}}}$$

and its mean first pressure derivative is

$$\beta'_{T\alpha x}=\frac{\beta^2_{T\alpha x}}{v_x}\sum_{j=1}^{n}\frac{\lambda_{xj}v_{xj}(1+\beta'_{T\alpha xj})}{\beta^2_{T\alpha xj}}-1.$$

In this new model, the powder is conceptually divided into a void space, V, and the idealized inert solid mixture (x), I, hence the name VI model. Since the void contains no mass, it cannot contain any internal energy, so all of the compressive work done on the void and solid will be contained in the solid. The specific volume and entropy of the solid material will be defined $v_x(P_x,T_x)$ and $s_x(v_x,T_x)$, respectively. The derivatives of the specific volume and entropy may be inserted in eq.(5) and the result equated with eq.(3) to yield,

$$\frac{\beta_{Tx}}{v_x C_{vx}}(P+\eta)dv_x=\left[\frac{P_x}{C_{vx}}-\frac{\Gamma_x}{v_x}T_x\right]dP_x+\left[\frac{\beta_{sx}}{v_x}-\frac{\Gamma_x}{v_x}\right]dT_x \quad (7)$$

where the definitions of the isothermal bulk modulus $\beta T=-v(\partial P/\partial v)_T$, the constant volume specific heat, $C_v=T(\partial s/\partial T)_v$, and the Grüeisen parameter were applied. The isentropic bulk modulus is defined

$$\beta_s=\beta_T+\frac{C_v\Gamma^2 T}{v}.$$

The distention ratio must jointly satisfy a specific volume and a pressure ratio definition[11], $\alpha=v/v_x$ and $\alpha=P_x/P$. The derivative of the specific volume condition is basically a restatement of the conservation of mass, $dv=v_x\,d\alpha+\alpha\,dv_x$. This derivative may be expressed in terms of pressure and temperature by inserting the derivative of $v_x(P_x,T_x)$ into it to yield,

$$\frac{dv+v_x d\alpha}{\alpha}=-\frac{v_x}{\beta_{Tx}}dP_x+\frac{C_{vx}\Gamma_x}{\beta_{Tx}}dT_x \quad (8)$$

In the VI powder mixture model and the VIR model, the distention ratio is described as a function of pressure[11],

$$\alpha = 1 + (\alpha_o - 1)\frac{(P_s^* - P)^2}{(P_s^* - P_e^*)^2} \quad \begin{matrix} \alpha_o & P < P_e^* \\ P_e^* \le P \le P_s^* \\ 1 & P_s^* < P \end{matrix} \qquad (9)$$

where $P_e^*$ is the elastic strength of the porous material and $P_s^*$ is again the crush-up pressure. Now a system of two equations, eqs.(7) and (8), and two unknowns, $dP_x$ and $dT_x$, exists which may be numerically solved utilizing a fourth order Runge-Kutta scheme in conjunction with the conservation of mass and momentum equations which provide the overall dv at each time step and eq.(9). During the pore collapse process, a convergence criteria is applied to check the dual distention-ratio definitions for convergence[2]. If the distention-ratio definitions do not agree with in a $3-5\%$ limit, the two values are averaged and the numerical step is repeated until convergence is achieved. This calculation is performed in conjunction with the hydrocode AUTODYN[12] to take advantage of the ability of this hydrocode to combine Eulerian and Lagrangian coordinate systems and utilize interactive rezoning of the mesh. The detonating nitromethane was modeled with a JWL equation[13] in Eulerian coordinates, the 304 SS with a $U_s - u_p$ equation[10] in Lagrangian coordinates, and the powder with the VI model in Lagrangian coordinates. The double walled structure of the capsule was included and the properties given in Table 1 were used in this calculation.

Figure 3(a) – (d) shows the calculated temperature and pressure contours in the Ti-Al mixture at sequential times for a crush-up pressure of 6 GPa. The Mach reflection grows in strength and width as it propagates through the powder. The high residual temperature, observable in Figure 3(d), is concentrated along the Mach stem. The region where the residual temperature is greater than the melting temperature of the aluminum, 933 K at ambient pressure, corresponds to the reacted region observed in the recovered specimen[7].

Comparing the 2-DL and VI powder mixture model calculations, Figure 2 and 3(d), the difference in the initial capsule structure places the Ti-Al at different coordinates, and some difference in mach stem

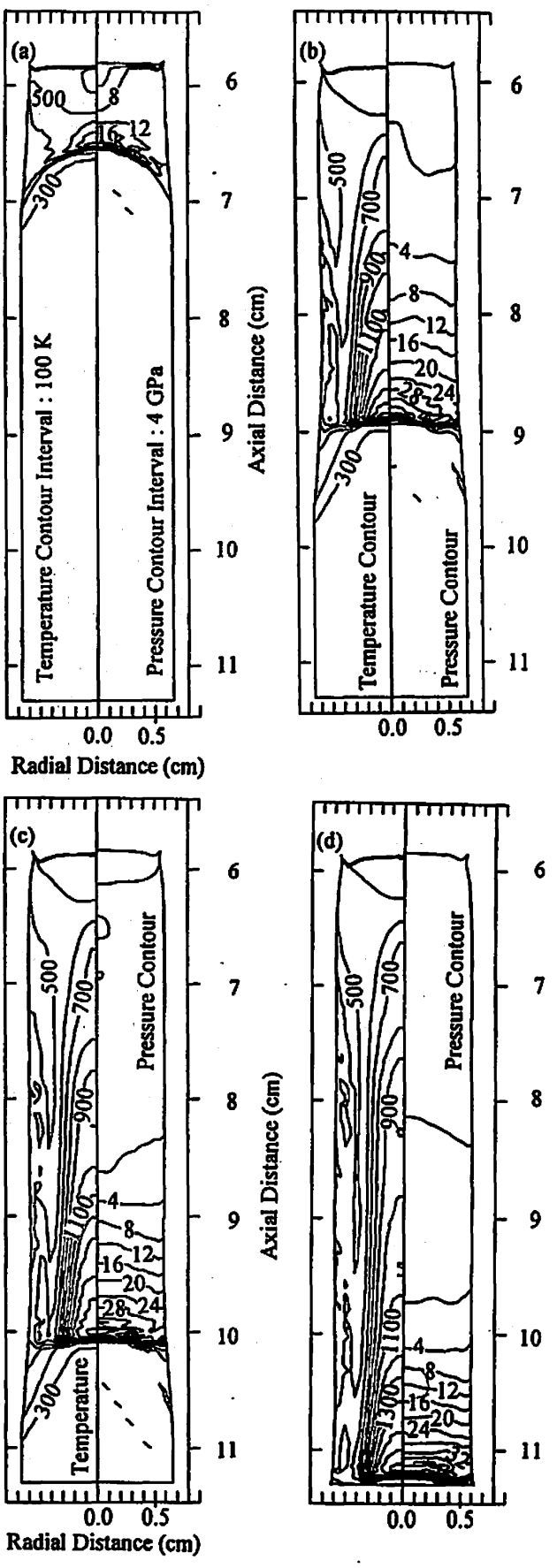


Fig. 3 Pressure and temperature contours in the powder mixture as calculated with the VI powder mixture model on AUTODYN at (a) 12.4 μsec, (b) 16.4 μsec, (c) 18.2 μsec, and (d) 20 μsec

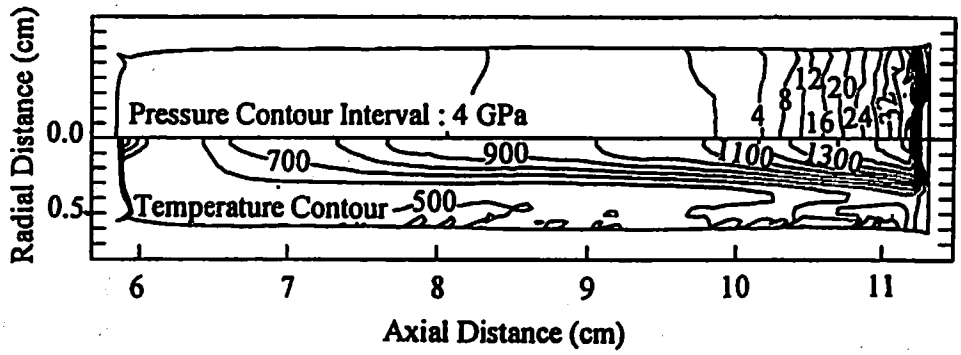


Fig. 4 Pressure and temperature contours at 20$\mu$sec in the powder mixture as calculated by the VIR model on AUTODYN

formation and propagation was evident due to the delay imposed by the collapsing double wall of the capsule. The pressure contours are similar as the mach reflection reaches the end of the powder sample; however, the temperature contours differ significantly. This difference is due to the assumptions concerning the Grüeisen parameter or Grüeisen ratio, $\Gamma/v$, remaining constant and the use of two different schemes to calculate the temperature, i.e. calculating the temperatures from the internal energy or directly from the first and second law of thermodynamics."

2.2.2 VIR Model

The final model that will be used to model the shock wave propagation is the VIR model[2] in combination with the hydrocode AUTODYN[12]. This reactive powder mixture model is capable of including chemical reactions in each subsystem and allows separation of the individual constituents into two subsystems with heterogeneous distribution of the pore collapse energy to simulate hot-spots and subsequent heat transfer to the "cold" subsystem. However, for this case, the pore collapse energy was assumed to be evenly absorbed and no reactions have been included so that the results will be comparable to the 2−DL and VI models. For this use, the notable difference between the VIR model and the previous two is that the individual constituents are each treated with independent EOS. Thus, each constituent responds to the pressure and temperature then the material properties of the mixture are calculated at each pressure-temperature step in the numerical solution.

The VIR model was applied in the same configuration on AUTODYN[12] and the pore collapse was described by the same polynomial equation, eq.(9), as in the VI powder model. The properties listed in Table 1 for the 304 SS and JWL model[13] were again used for the calculation and the individual constituent properties were used for the Ti-Al powder mixture. For the result shown in Figure 4, the pore collapse pressure was also set to 6 GPa. The pressure and temperature contours in the Ti-Al mixture and the propagation distance are similar to those shown in Figure 3(d). This shows that, in this Ti-Al experiment, the individual treatment of the constituent EOS is similar to treating them as a simple ideal mixture with one EOS. If shock-induced reactions had been included in the VIR model, this comparison would not have been valid.

## 3. Conclusions

All three models, 2−DL, the VI powder model, and the VIR model, yield very similar results for the pressure contours in the Ti-Al powder mixture; however, there are some differences in the temperature contours as calculated by the 2−DL model due to different assumptions in the calculation. This shows that the traditional method of modifying only the EOS and then calculating the temperature from the internal energy vs. the proposed linking of the conservation of energy and the second law of thermodynamics to directly calculate the temperature produce similar results for an inert powder mixture in the pressure regime. However, the temperature calculations differ significantly between the two schemes. It is difficult to definitively determine which scheme is better for calculating the temperature profiles but, the profiles obtained from the latter method seem to more closely fit the observed experimental results. This study also shows that the individual vs. ideal mixture treatment of the constituent EOS gives similar

results for an inert powder mixture.

For the VI and VIR models, the calculated residual temperatures in the Ti-Al sample are equal to or greater than the melting temperature of the aluminum in the area of the Mach stem which corresponds to the observed reaction region in the recovered specimen. This indicates that the observed reaction could be a "shock assisted reaction" but does not rule out the possibility that is was a "shock-induced reaction."

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## Ti/Al粉末中の爆発衝撃現象の数値解析


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SUS 304ステンレス鋼管でできた衝撃処理用カプセルに密閉したTi/Al混合粉末中を伝播する衝撃波について古典的なMie-Gruneisen，ここで提案されたVI(空隙－不活性物質)，BennettとHorieによるVIR(空隙－不活性物質－反応性物質)の3種類のモデルにより数値解析を行った。解析では，著者の田中による2DLコードとAutodynの2種類のコードが使用された。その結果，爆薬の爆轟速度と粉末中の衝撃波伝播速度の違いにより混合粉末中に弱マッハ反射が形成されることがわかった。Mie Gruneisen式とVI及びVIRモデルでは計算される温度に大きな違いが生じた。計算の結果，衝撃圧縮状態から大気圧状態まで解放されたときの残留温度(residual temperature)のプロフィルは実験で観測された反応に重要な影響を与えていることが判明した。



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