

Generation of isentropic compression by use of multi-layer composite flyer and its influence on system thermodynamics: A simulation study

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Abstract. Recently the possibility of achieving quasi-isentropic compression using functionally graded materials, in both gas gun and explosive driven systems was explored by hydrodynamic simulations. In the current paper, we show that multi-layered composite flyer with progressively increasing shock impedances, referred to as graded density impactor (GDI), has the potential to enable increased flexibility in suitably tailoring the applied-pressure profiles, further relaxing constraints on the thermodynamic path of compressed material. Present simulation study pertaining to constant velocity impact of GDI reveals that linear ramp pulses of different pressure rise times, with comparable peak values can be realized only by changing the layer thicknesses of a particular GDI. We report generation of three different slope ramp pulses by five layer GDI made of PMMA, Al, Ti, Cu and Ta with different set of thicknesses obtained by genetic algorithm based optimization technique. Generation of long duration (μs) isentropic pressures using discrete GDI is a significant step, since it is devoid of fabrication difficulties of ultra-thin lamellae of FGM. Signatures of isentropic compression of a thin Cu target under different slope ramp loadings are identified from basic thermodynamic aspects in terms of temperature rise and entropy production. It is shown that that extent of entropy increase is closely related to the slope of ramping pulse. Further, a physical model has been constructed to determine approximate time profile of pressure pulse generated by equal layer-width GDI.

1. Introduction

Investigation of material properties at extreme thermodynamic conditions, i.e. ultra-high pressures at any temperature is of interest to many fields dealing with High Energy Density [1]. By shock or isentropic techniques one is able to realize dynamic high pressures [2–5]. Main difference between the two approaches is that there is an abrupt increase of sample temperature by strong shock compression, which is in contrast to relatively low temperature rise for isentropic or quasi - isentropic methods [2]. Isentropic methods offer a practical way for comprehensive determination of material response and EOS properties in a broad range of phase diagram. Shock - induced high pressures can be generated by impact of high velocity flyer plates, which has inherent limitations of significant target heating. In order to modify the facility for low temperature EOS measurements, one can either use continuously changing *functionally graded materials* (FGM) or discrete *graded density impactors* (GDI) so as to achieve shock-less, low entropic compression. Isentropic wave was first generated by impactors made of varying density powders [6]. Recent advances in fabrication of FGM have opened a new front in generating smooth, continuous isentropes [7, 8].



We have explored the possibility of achieving isentropic compression using continuously changing FGM, in both gas gun and explosive driven systems by hydrodynamic simulations [9]. However, fabricating these thin lamellae of FGM requires high precision in respect to gradation of their physical properties one seeks for. In this regard, use of multi-layered impactor made of commonly available materials has shown increased flexibility in suitably tailoring the applied-pressure profiles. Sandia laboratory has reported the experimental realization of shaped pressure pulse using seven-layer GDI [10]. Nevertheless, time profile of measured velocity pulse showed sharp shock jumps. Generation of isentropic compression using impactor made of eight different material layers, whose shock impedance are in progressively increasing order has been examined in our earlier work [11]. In the current paper we have employed five distinct layers, namely PMMA, Al, Ti, Cu and Ta, in GDI to produce isentropic waves. The simulation study pertaining to constant velocity impact, similar to that of gas gun, of the said GDI reveals that linear ramp pulses of different pressure rise times, associated with comparable peak pressures, can be realized only by changing the layer-widths of a particular composite flyer. The layer thickness combinations required for a particular ramp pulse is determined by optimization technique. Signatures of isentropic compression under different slope ramp loading to Cu target are identified from basic thermodynamic aspects, paying particular attention to temperature rise and entropy production. Study reveals that extent of entropy increase is closely related to the slope of applied ramping pulse.

2. Simulation model - Determination of layer thickness

To that end, we consider above mentioned five-layer GDI (7 mm thick), being launched at 1 km/sec velocity toward a 5 mm thick Cu plate, followed by 1 cm thick LiF window used for diagnostic purposes. Except for FGM being replaced by GDI, the simulation system is same as reference [9]. The EOS parameters of layer materials, target and window are adopted from reference [12]. In order to generate isentropic pressure profile at target surface, GDI layers are arranged in such a way that lowest density layer faces the target side, rear end has highest density; and density of in-between layers are in increasing order.

Pressure gradient created in a medium by high velocity impact causes spatial and temporal change in material density, which, in turn, affects pressure distribution in a self-consistent manner. The resulting hydrodynamics, characterized by four variables: fluid velocity, density, fluid pressure, and specific internal energy, is described by three conservation equations of mass, momentum and energy, and an appropriate EOS. For the present simulation study, we have used earlier developed 1D Lagrangian hydrodynamic code [9]. Further, hydro code has been coupled with genetic algorithm program, PIKAIA [13] for optimization of thermodynamic quantities or hydrodynamic flow variables. We have found layer-widths of certain GDI by genetic algorithm based optimization calculation for arriving at linear ramp pulses. In order to do so, first we choose the slope m of desired pressure profile, $p_{fn}(t) = m * t$ and pulse rise time, t_1 . Hydro calculation is carried out with thicknesses of four layers being determined from four random numbers, fifth one is calculated from total width of GDI. Next, for every time step the difference between hydrodynamic pressure and functional pressure is calculated. If N time steps are followed to reach t_1 , then mean residual square (MRS), σ is defined as

$$\sigma = \frac{1}{N} \sum_{t=0}^{t_1} [p_{hyd}(t) - p_{fn}(t)]^2, \quad (1)$$

where $p_{hyd}(t)$ is simulated hydrodynamic pressure at first mesh of GDI (target end). In order to minimize MRS, we have chosen $f_{fit} = 1/\sigma$ as a suitable fitness function for optimization routine. Hence, by minimizing σ or maximizing f_{fit} we finally arrive at optimized layer widths for which $p_{hyd}(t)$ coincides with $p_{fn}(t)$ for $t \leq t_1$. This is achieved after few generations provided

a large number of populations are followed in each generation. By employing the above method, we have generated three different pressure pulses with slopes $m = 0.11$, $m = 0.2$ and $m = 0.3$. With the experience of earlier study that peak pressure achievable by similar experimental setup employing continuous FGM is about 0.22 Mbar, rise times for three pulses are chosen to be $t_1 = 2.3 \mu s$, $1.4 \mu s$ and $0.8 \mu s$ respectively. The layer-widths, $x_i : i = 1, 5$, obtained by this coupled optimization-hydro simulation are listed in table 1. Shock impedances, $Z_i (= \rho_i * C_i)$ of the materials are also listed. Since the layer-widths found are of mm order, GDI of this kind can be made by stacking one layer over the other, as has been done in experimental study of [10]. Hereafter, three sets of GDI with different layer-width combinations will be referred to

Table 1. Optimized layer-widths (in cm) for three different GDIs.

Material	ρ_i (gm/cc)	Z_i	x_i (GDI-1)	x_i (GDI-2)	x_i (GDI-3)
PMMA	1.19	0.31	0.1484	0.0801	0.0538
Al	2.79	1.48	0.1273	0.0958	0.0698
Ti	4.53	2.26	0.1724	0.09	0.0775
Cu	8.93	3.48	0.0767	0.0872	0.3489
Ta	16.66	5.83	0.1752	0.3469	0.15

as GDI-1, GDI-2, and GDI-3 respectively. Further, layer-widths in GDI-1 observed to follow quadratic variation of density along its thickness, in consistence with our earlier finding with FGM flyer.

3. Applied pressure profile

The influence of multiple reflections at material interfaces on shock wave propagation in layered composites can be illustrated by time history of pressure profiles. Figure 1 compares time variation of pressures applied to Cu surface by either of the constituent material (each of 7 mm thickness), with that produced by GDI-1. The profile obtained by GDI-1, up to peak (0.25 Mbar), is reminiscent of a linear ramp pulse of isentropic wave. The dashed line in the figure shows linear fit, $p(t) = 0.11 * t$ of data up to $2.3 \mu s$, i.e., the time when peak occurs.

Applied pressure profiles generated by any single material flyer consists of initial sharp shock jump, followed by a plateau region (seen with numerical oscillations) indicating attainment of equilibrium, and release wave that decompresses the shocked state. Duration of plateau region is determined by flyer thickness and impact velocity of shock loading. Peak pressure realized with lowest (PMMA) and highest (Ta) impedance materials are lowest and highest respectively. Appearance of plateau region in case of GDI loading depends on details of multiple reflections between different layers. Note that pressure pulse produced by GDI-1 does not contain any plateau, rather it exhibits smooth loading (compression) and unloading (release) waves. However, with appropriate geometrical length scale and mechanical properties of each component layer, plateau region may become more prominent as shown below. It is clear from figure 1 that slow rise in pressure for GDI impact does not reduce peak value significantly.

In figure 2, we have shown the time history of applied pressure obtained by GDI-2 and GDI-3 with layer widths given in table 1. It is observed that pulse rise time, $t_1 \approx 1.4 \mu s$ of GDI-2 is less than that for GDI-1. This is expected as width of Ta flyer has been increased from 1.7 mm of GDI-1 to 3.4 mm in GDI-2 case. Thick Ta layer also induces an almost plateau region before finally releasing at $2.5 \mu s$. In case of GDI-3, marginally lower peak pressure associated with much shorter rise time ($t_1 \approx 0.8 \mu s$) is observed. The waveform in this case has an initial ramp with slope $m = 0.3$, subsequent sharp fall followed by oscillatory region, which is a direct consequence of shock reflection at Cu-Ta interface. The dashed and dotted curves of figure 2 correspond to linear fits $p(t) = 0.2 * t$ and $p(t) = 0.3 * t$ of $p_{hyd}(t)$ vs t data generated with GDI-2

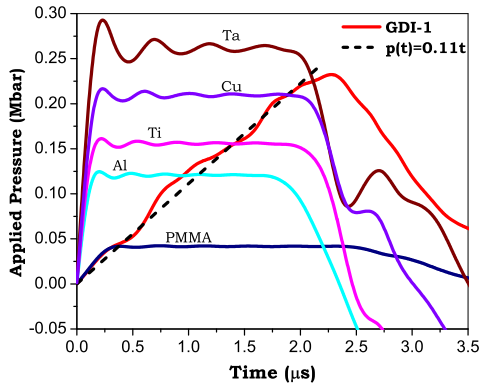


Figure 1. Time profile of pressure pulse applied to Cu target by GDI-1. Dashed line is the linear fit, $p(t) = 0.11 * t$. Pressure profiles generated by 7 mm thick individual material of GDI are also shown.

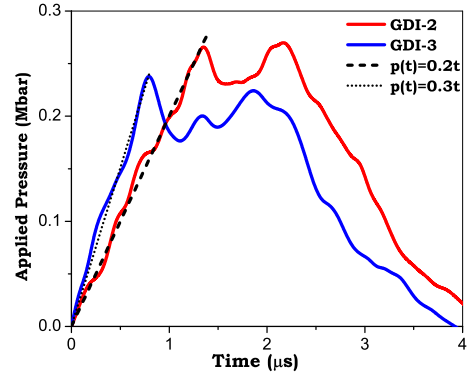


Figure 2. Time profile of pressure pulse applied to Cu target obtained by GDI-2 and GDI-3. Dashed and dotted lines refers to linear fits: $p(t) = 0.2 * t$ and $p(t) = 0.3 * t$.

and GDI-3, up to their respective rise times. Ideally, for realizing steeper pulses the widths of front and successive layers should be reduced thereby reducing total thickness of GDI. However for fixed flyer thickness, widths of front layers are decreased at the cost of increasing widths of rear end layers (Cu & Ta). This leads to deviation from ideal ramp beyond pulse rise time, but helps in maintaining target pressure before unloading.

4. Effect of various ramp waves on target thermodynamics

In order to characterize isentropic compression from thermodynamic point of view, next we investigate the temperature rise and entropy increase in the target, compressed by thus generated ramp pressures. Thermodynamic variables of the compressed state can be estimated theoretically by the knowledge of measured shock wave parameters along Hugoniot. From our earlier work [11], we can express temperature along Hugoniot as:

$$T_H(V) = \chi(V) \left\{ T_0 + \int_{V_0}^V \frac{f(V')}{C_V(V', T)\chi(V')} dV' \right\}, \quad \chi(V) = \exp \left[- \int_{V_0}^V \frac{\gamma(V')}{V'} dV' \right] \quad (2)$$

In the above, temperature along the isentrope can be recognized as $T_i = T_0\chi(V)$, where T_0 is the material temperature at initial volume V_0 . The functional form of $f(V)$ is determined from Hugoniot state (p_H, V) as

$$f(V) = \frac{1}{2} \left[(V_0 - V) \frac{dp_H(V)}{dV} - p_H(V) \right], \quad p_H(V) = \frac{C^2(V_0 - V)}{[V_0 - S(V_0 - V)]^2}. \quad (3)$$

Temperature at any arbitrary $(p - V)$ state is obtained from internal energy relation $dE/dT = C_V(V, T)$. Assuming classical value of constant specific heat C_V , temperature at any off-Hugoniot state is simplified to

$$T(V) = T_H(V) + \frac{E(V) - E_H(V)}{C_V}. \quad (4)$$

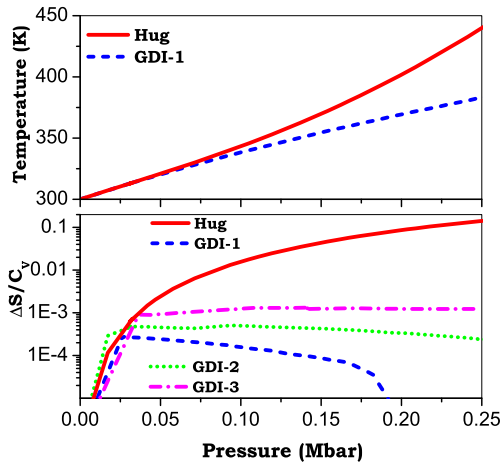


Figure 3. Variation of target temperature rise (Top) and entropy production (Bottom) with target pressure.

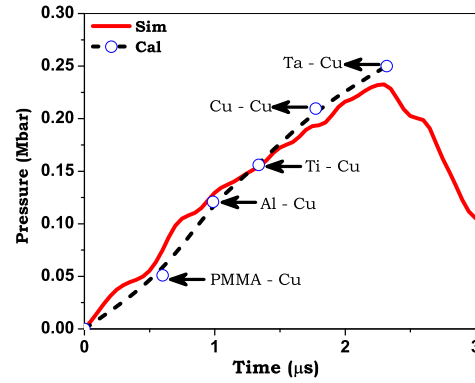


Figure 4. Pressure profile generated by equal width GDI layers. Symbols represent calculated ($p - t$) data obtained by impact of individual layer with Cu target.

The entropy increase ΔS , in going from an ideal isentrope, characterized by temperature T_i and entropy S_i , to any compressed state at same volume, identified by temperature T_f and entropy S_f , can be expressed as,

$$\Delta S = S_f - S_i = C_V \int_{T_i}^{T_f} \frac{dT}{T} = C_V \log \left(\frac{T_f}{T_i} \right). \quad (5)$$

If $T_f = T_H$, then equation 5 represents entropy increase along Hugoniot. ΔS would be zero for ideal isentrope. For quasi - isentropic case ΔS is usually a small number. figure 3 shows target temperature rise (top) as a function of target pressure. Solid line refers to Hugoniot simulated by impact of normal density flyer launched at different velocities providing different peak pressures. Dashed line displays result for isentrope generated by impact of GDI-1 at 1 km/sec. It is found that temperatures for all the three GDI cases are nearly same and hence are not shown separately.

Entropy production for three GDI cases is quite different as illustrated in bottom layer of figure 3. Here ΔS (in units of C_V) is plotted as a function of increasing pressure. The solid curve, corresponding to Hugoniot, lie much above GDI results. As pressure increases there is a steady increase in entropy production along Hugoniot, thereby increasing the extent of irreversible energy loss. Thus more energy goes into heating the material than compressing it. In contrast, entropy production for GDI induced isentropes is order of magnitude smaller and remains nearly constant up to final pressure. The entropy curves for all GDI induced isentropes exhibit an initial steep rise caused by the first shock, followed by essentially negligible contribution arising due to successive disturbances that elevates the pressure to final value. For GDI-1 with lowest slope ramp loading, entropy production is lowest and it is two orders of magnitude lower than Hugoniot. Moreover, plateau of the entropy curve for GDI-2 and GDI-3 cases lie much above GDI-1 value, indicating that lowest slope ramping is best option for isentropic compression.

5. Analytical Results

Next, we evaluate the approximate pressure profile realizable at a thin target on impact of multi-layer composite flyer at velocity v_i . After the impact of any layer of density ρ_i compressive

shock wave formed travels into the target with velocity u_{st} and into the projectile layer with a velocity u_{si} . Particle velocity of target, u_{pt} and impactor, u_{pi} to be determined are related by: $u_{pt} + u_{pi} = v_i$. In order to find the pressure and velocities after shock collision we adopt impedance matching approach at the interface. Exploiting Hugoniot EOS of materials to express pressure as $p = \rho(C + Su_p)u_p$ and continuity of pressures p_t and p_i at interface, we solve for u_{pt} and u_{pi} . Thus we arrive at analytical expressions for particle velocities and pressures as a function of speed v_i and C , S and ρ values of target and layer. Defining relative velocity of the projectile $v_{ri} = (u_{si} - u_{pi} - v_i)$, the time to travel a layer of thickness x_i is: $t_i = x_i/v_{ri}$. Total time of impact of all 5 layers is $t = \sum_{i=1}^5 t_i$. We apply this technique for successive impact of five layers with densities ρ_i . Figure 4 shows good agreement of simulated pressure profile (solid line) obtained for equal width five layer GDI with analytical results (dashed curve) of approximate time profile.

6. Conclusions

Results of hydrodynamics simulations using GDI for generating smooth isentropic waves, as obtained with FGM, are reported. Different slope ramp pulses are realized by changing width of individual layers of same 5-layer GDI, however, maintaining the total thickness. Generation of ramp pulses with relatively thick discrete density layers is rather easier from design point of view, since it is devoid of fabrication difficulties of ultra-thin lamellae of continuous density FGM impactor. Signatures of isentropic compression are identified from thermodynamic properties. Finally, target entropy increase is shown to be related to ramping slope.

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