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Fabrication and Design of Multifunctional Energetic Structures Using Gradient Architectures

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ABSTRACT

The use of gradient architectures for multifunctional energetic structures is investigated using Twin Screw Extrusion (TSE) processing technology that has been configured for fabricating graded materials. It is demonstrated that polymer composites with both radial and axial gradients can be produced using this technology. A concurrent design effort is also undertaken to determine the optimal gradient architecture for a multifunctional energetic structure using the properties of the TSE processed energetic materials in structural and ballistic performance analyses. As an example case, a cylindrical propellant grain with a single perforation and a radial gradient is analyzed. It is determined that the maximum thrust can be increased by 40% and the total impulse can be increased by 73% using a gradient architecture that varies linearly from a normalized radius of 0.82 to 1.

INTRODUCTION

To realize advancements in energetics that can reduce weight and enhance performance, there is a need to design novel energetic materials and structures that are capable of multifunctional performance. For example, new propellants concepts are being developed that focus on optimizing the integration of conventional energetic materials into energetic systems using functionally graded materials concepts [1]. These concepts take advantage of Twin Screw Extrusion (TSE) processing, a continuous manufacturing technology, for producing high performance energetic materials using thermoplastic elastomeric (TPE) binders [2]. The resulting graded propellants have a variation in burn rate that can be used to tailor the ballistic performance of a solid propellant to behave more like a liquid. It also has the potential for varying other physical characteristics, such as mechanical properties, in addition to the burn rate. By considering the mechanical and ballistic performance, it is possible to use functionally graded materials concepts to develop multifunctional energetic structures.

In this paper, the grading of a TSE processed energetic material for the development of a multifunctional energetic structure is investigated. Polymer composites with gradient architectures are fabricated as inert simulants of composite energetic materials. Concurrently, prior measurements of mechanical and burn rate properties of homogeneous compositions for these formulations are used to propose design models for multifunctional performance predictions. Both mechanical and ballistic performance are analyzed for a cylindrical propellant grain with a single perforation, where the pressure in the perforated cavity produces mechanical stresses that are sufficient to exceed the mechanical strength of the propellant material. Using the mechanical strength as a constraint on the design of the grain, the optimal gradient architecture that maximizes the thrust produced by the grain can be determined.

TSE PROCESSED ENERGETIC MATERIAL

The manufacturing of composite energetic materials has been traditionally performed using batch processing. Recently, TSE processing has been explored to continuously manufacture military propellants using TPE binders to control viscosity during processing [2]. In addition to military propellants, TSE processes are utilized to manufacture a world of consumer and industrial goods from snack foods and medical tubing to plastic pellets. For military propellants, TSE processed energetic materials exhibit strengths and burn rates that are superior to batch processed material. These strengths are approximately 225 MPa for a standard AP formulation, which is approximately 50% greater than observed for identical batch-processed formulations. The burn rates are approximately 50% greater than observed for identical batch-processed formulations. Formulations usually vary between 78 vol. % and 87 vol.% solids loading, which has a more significant effect on the burn rates than on the mechanical behavior. Therefore, the mechanical properties can be assumed constant, while the variation in burn rates will become the focus of the FGM concept for the multifunctional energetic structure.

PETITE ENSEMBLE MODEL BURN RATE PREDICTIONS

For determining the material gradient and distribution in a propellant, a model is required to describe the combustion process. Based on the prediction of this model, the performance of the multifunctional propellant grain can be optimized. For this investigation a Petite Ensemble model (PEM) for steady-state combustion is used [3]. The PEM is based on a statistical treatment of the propellant surface with multiple flame structure centered about characteristic oxidizer particles. This model can be summarized by the following equations:

$$F_d = \frac{1}{(2p \ln s)^{1/2}} \exp\left[-\frac{1}{2}\left(\frac{\ln D_o - \ln \bar{D}_o}{\ln s}\right)^2\right] \quad [1]$$

$$\bar{r} = \int_{D_o} \frac{r_d F_d}{a_d} d(\ln D_o) \quad [2]$$

$$R_p = \frac{1}{\bar{r}} \int_{D_o} \frac{R_{p,d} r_d F_d}{a_d} d(\ln D_o) \quad [3]$$

$$R_v = \frac{1}{\bar{r}} \int_{D_o} \frac{R_{v,d} r_d F_d}{a_d} d(\ln D_o) \quad [4]$$

where F_d is the overall oxidizer distribution function, D_o is the oxidizer particle diameter, $\bar{D}_o$ is the mean oxidizer particle diameter, s is the oxidizer distribution function mode width parameter, $\bar{r}$ is the composite propellant mean burning rate, r_d is the burn rate for a pseudopropellant, a_d is the pseudopropellant oxidizer mass fraction, R_p is the composite propellant pressure coupled response function, $R_{p,d}$ is the pseudopropellant pressure coupled response function, R_v is the composite propellant velocity coupled response function, and $R_{v,d}$ is the pseudopropellant velocity coupled response function. PEM predictions of the variation in burning rate with composition for TSE processed energetic materials can be seen in *Figure 1*. For compositions with solids loading ranging from 78 vol. % to 87 vol. %, the predicted burn rates can vary by 50%. Using these burn rate predictions, it is possible to inversely determine the compositional variation associated with the gradient architecture that optimizes ballistic performance in a multifunctional energetic structure

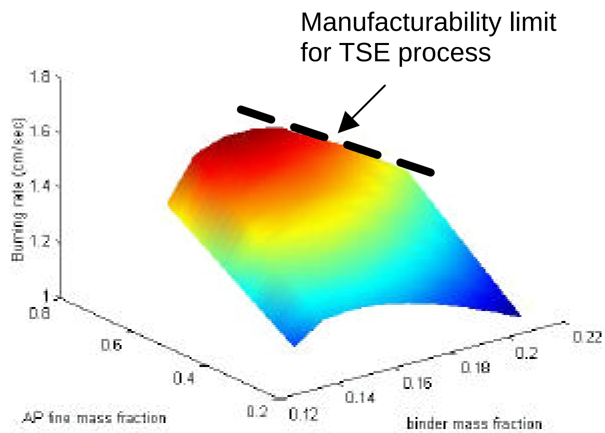

Figure 1. PEM prediction of variation in burning rate with composition for TSE processed energetic materials

GRADED ENERGETIC MATERIALS

While composite energetic materials for rocket motor applications are typically processed homogeneously using batch techniques, the novel continuous processing technology known as Twin Screw Extrusion (TSE) has been recently demonstrated to produce higher quality products. However, the true potential of the continuous processing aspects of the technology have yet to be fully realized. In addition to process safety, economy, flexibility, and quality, the most interesting feature of TSE is the ability to produce continuously graded architectures. These graded architectures have a significant impact on direct concepts for solid rocket motor applications.

Conventional solid rocket motors consist of a uniform propellant composition throughout. They are typically produced this way on purpose, necessitated by safety and performance considerations. The consequence of uniform composition is uniformity in burning rate behavior, and thus the thrust performance is very predictable. This performance results in a constraint on design concepts for rocket motors, where the only design variables become the topological characteristics of the motor. Ideal rockets should have a controllable thrust, which is true for liquid propellants where the fuel is metered to the combustion chamber. However, liquid propellants are not well suited for many rocket motor applications due to higher needs for storage and handling safety and shelf-life limitations among others.

There is a desire for solid rocket motors that can exhibit a variable burning rate profile while in flight. The answer to this is a rocket propellant that employs FGM concepts. Thinking of the propellant as a long cylinder, the composition would be graded in the length direction (*Figure 2*). For an end-burning type rocket, there would be one propellant formulation, identified as composition A, at the ignition with a particular burning characteristic. At some point during flight, there would be a point of transition to a second type of propellant, identified as composition B, with a different burning characteristic that was specified by the designer to maximize the rocket's potential to reach its target. As shown in Figure 2 the volume of composition B at one end is zero and 100 percent at the other. At some point between the two, there is a continuous and smooth transition from one to the other.

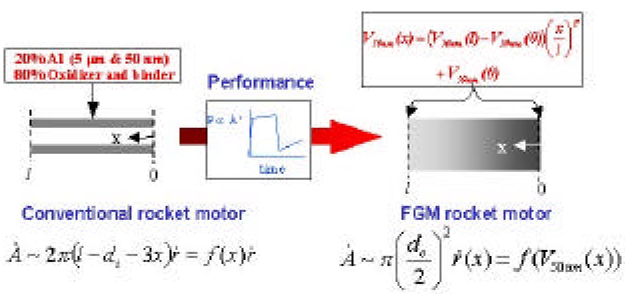

Figure 2. Comparison of conventional solid rocket motor concept with FGM concept

The TSE process is naturally suited to produce this type of gradient from one composition to another. Operating a twin screw extruder at one steady condition and dynamically changing the ingredients to produce a new formulation will result in the extrudate changing from the original composition to second one. Because of the inherent backmixing in a twin screw extruder, an abrupt change in ingredients results in a more gradual change in the composition of the extruded product. There are several ways to achieve this for a rocket propellant. One simple idea is to decrease the volume of oxidizer that reduces the burn rate. However a more effective idea is to change the ratio of coarse to fine sized particles. A combination of the two coupled with a process change, such as extruder screw rpm, will be studied. In this way, the continuous process is especially well suited to producing Functionally Graded Materials (FGMs). In contrast the batch process is incapable of producing a smooth and continuous transition.

In addition to variations in the ingredients, the operating conditions of the TSE can also be varied. This can be used to control the extent and composition profile for the gradient architecture. It will also be possible to vary the screw configuration of the extruded to alter the characteristics of the gradient architecture. The effects of dynamic variations in ingredients and operating conditions for a given screw configuration have been modeled in order to predict the evolution of graded architectures in the TSE process [1].

TSE PROCESSING OF GRADIENT ARCHITECTURES

The TSE process is a continuous type in that the twin screw extruder will produce a product as long as the ingredient supply is maintained. Because this type of process has so many advantages over batch type, it has found widespread utility across diverse industries. For most however the advantages are universal: economy, quality, environmental, flexibility, and safety. In the case of energetic materials, all these advantages have been proven. Some of these illustrate why the twin screw extruder shows great promise for producing graded materials.

To understand the TSE process, a description of the equipment is necessary. The extruder consists of two screws, typically fully intermeshing, which run through temperature-controlled barrels. The barrels are modular in design and specialized for feeding solid and liquid ingredients, vacuum, or other functions. They are interchangeable allowing a configuration best suited to a particular process. Furthermore the screws consist of various segmented elements that slide onto the screw shafts allowing for customizable screw designs. Like the barrel sections, various screw geometries are available which are utilized for conveying ingredients, gentle and high shear mixing, devolatilization, and many others. Hence the mixer is highly configurable and thus very flexible allowing for the optimization of many types of processes. In less than a work shift, the mixer can be reconfigured for a completely different product.

This flexibility lends itself to facility expenditure savings. As with the case of naval gun propellants, the discrete batch process required a number of individual process steps, each with its own facility, equipment and operators. The continuous process with a twin screw extruder eliminates some steps and allows the rest to be combined. The result is a great reduction in the number of facilities required and one continuous operation. In that the mixing/extrusion/cutting operation is remotely operated, the safety of the process is much greater by reduced operator exposure to hazards and reduced quantities in a mixing state at any point in time.

Furthermore the continuous process yields a more consistent product thus improving overall quality. There is significantly less variation in material, and the efficiency of mixing is better than batch methods. The process lends itself to on-line analysis allowing for the quick detection of anomalous conditions or material automatically diverting it to waste. In the batch process this is impossible until later in the production after a large quantity of potentially bad product has been made.

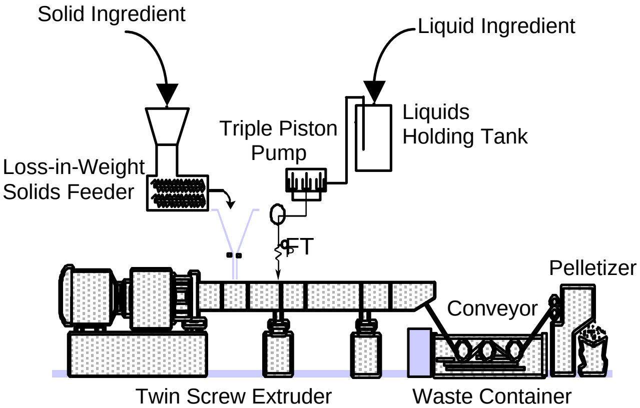

Figure 3. Twin-screw extrusion process

The extruder is only the heart of the process (*Figure 3*). The process is supported by various ingredient feeders. The quality of the extruded product is directly influenced by the accuracy of the ingredient addition. For this reason only the most accurate feeding technologies are utilized. These commonly include loss-in-weight control for solid ingredients and flow metering control for liquids. Additionally, there are temperature control units for the extruder barrels and a process control system for the facility which are not shown in the figure.

As mentioned previously, changing the ingredients, operating conditions, and screw configuration can affect the evolution of gradient architectures. This is demonstrated in *Figure 4* using inert simulants of composite energetic materials consisting of Potassium Chloride and an Engage^{TM} polymer from Du Pont. From this figure, it can be seen that the TSE process is capable of producing gradients in both the axial and radial directions. Although the TSE process can provide three-dimensional control over material variation, which is essential for three dimensional burning surfaces, a much simpler two-dimensional burning surface will be investigated in the following performance analysis.

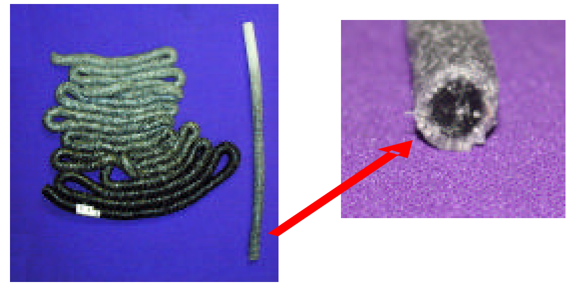

Figure 4. Graded composites comprised of inert simulants processed using TSE

MULTIFUNCTIONAL PERFORMANCE MODELING OF FUNCTIONALLY GRADED PROPELLANTS

Mechanical Performance

In order to model the mechanical performance, an example case of a rocket motor grain with a single perforation and inhibited ends is analyzed (*Figure 5*). Burning occurs on only the inner surface of the grain, while pressure develops in the perforated cavity. A rocket motor casing surrounds one end of the grain, which enables thrust force to be generated. The subsequent pressure loading generates stresses in the grain and the casing that can be sufficient to fail either one. To predict the effects of the cavity pressure on the mechanical performance on the grain and casing, the system can be treated as two concentric axisymmetric cylinders. Both the behavior of the grain and the casing can be treated as linearly elastic. While the grain can experience fairly large strains (<15%), an infinitesimal deformation solution can still provide a good approximation of the stress state in the grain. The stress state, $(\sigma_{rr},\sigma_{\vartheta\vartheta},\sigma_{zz})$ can be predicted using the following solution to Lame's problem [4]:

$$s_{rr} = \frac{p_i R_i^2 - p_o R_o^2}{\left(R_o^2 - R_i^2\right)} + \frac{R_i^2 R_o^2 \left(p_o - p_i\right)}{r^2 \left(R_o^2 - R_i^2\right)} \qquad [5]$$

$$s_{qq} = \frac{p_i R_i^2 - p_o R_o^2}{\left(R_o^2 - R_i^2\right)} - \frac{R_i^2 R_o^2 \left(p_o - p_i\right)}{r^2 \left(R_o^2 - R_i^2\right)} \qquad [6]$$

and for Plane Strain:

$$s_{zz} = n\left(s_{rr} + s_{qq}\right) = \frac{2n\left(p_i R_i^2 - p_o R_o^2\right)}{\left(R_o^2 - R_i^2\right)} \qquad [7]$$

where R_i is the cavity radius, R_o is the external radius of the grain, p_i is the internal pressure, p_o is the external pressure, and R is the radial position in the grain.

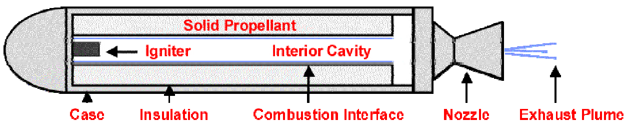

Figure 5. Rocket motor with a grain containing a single perforation for multifunctional performance modeling.

For these multifunctional energetic structures, the desire is to replace conventional casing materials with ones that are more compliant and lightweight. These new casing materials will not provide as much constraint to the propellant grain as conventional casing materials, thereby placing a greater emphasis on the structural characteristics of the propellant. The critical stress will then become the hoop stress for the propellant grain, $\sigma_{\vartheta\vartheta}$, which will initial radial cracks that will cause the rocket to explode. It is therefore this component that will be of interest in the modeling analysis, and will need to be less than the critical stress for the propellant material. Therefore, the internal pressure generated by the burning process will dictate the pressure that must be applied to the outer boundary of the propellant grain by the casing in order to prevent failure. For a failure stress, σ_f, the critical internal pressure, p_{crit}, can be determined as a function of the radius for the burning internal cavity, R, as follows:

$$p_{crit} = \frac{-\left[\frac{-(R_o)^2}{\left[\left[(R_o)^2 - R^2\right]\right]}\cdot p_o + \frac{1}{\left[R^2 - (R_o)^2\right]}\cdot p_o\cdot (R_o)^2 - \sigma_f\right]}{\left[\frac{(R_o)^2}{\left[\left[(R_o)^2 - R^2\right]\right]} - \frac{1}{\left[R^2 - (R_o)^2\right]}\cdot R^2\right]} \quad [8]$$

Assuming an external pressure equal to the failure stress of the propellant, a plot of the critical pressure normalized by the external pressure versus the radius of the burning internal cavity normalized by the outer radius can be seen in *Figure 6*. It is clear from this figure that the cavity pressure must decrease as the cavity radius approaches the outer radius. To determine how this cavity pressure is related to the buring rate of the propellant, a ballistic analysis of the rocket motor performance must be performed.

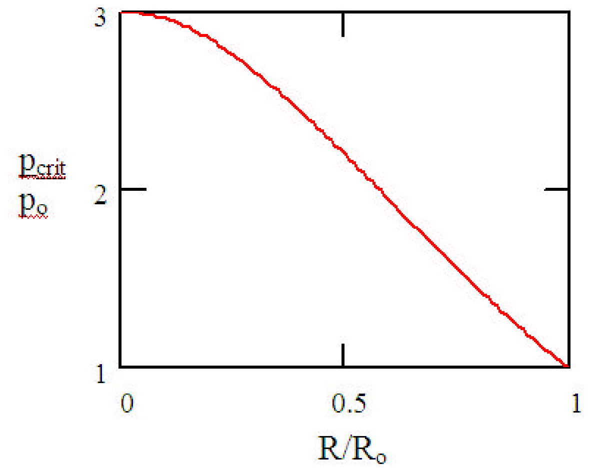

Figure 6. Plot of the normalized critical pressure versus the normalized burning cavity radius

Ballistic Analysis of Rocket Motor Performance

To predict the performance of rocket motor with a grain containing a single perforation, a conventional ballistic analysis can be employed. For steady state burning, the equilibrium cavity pressure, P_i, for the motor can be determined from a balance of mass analysis assuming negligible mass storage as follows [5]:

$$\dot{W}_g = \dot{W}_d \quad [9]$$

$$r_b\, A_s\, ?_p\, g_o = C_D\, P_i\, A^* \quad [10]$$

$$r_b = a\, P_i^n \quad [11]$$

$$C_D = g_o/c^* \quad [12]$$

where $\dot{W}_g$ is the mass flow rate of the burning propellant,

$\dot{W}_d$ is the nozzle mass exhaust rate, r_b is the burning rate of the propeallant, a is the burn rate coefficient, n is the burn rate exponent, A_s is the internal surface area of the cavity, r_p is the density of the propellant, A^* is the nozzle throat area, C_d is the discharge coefficient, c^* is the characteristic velocity of the nozzle, and g_o is the gravitational constant. The equilibrium cavity pressure is therefore given by:

$$P_i = (a\, ?_p\, A_s\, c^*/A^*)^{1/1-n} \quad [13]$$

In equation [13], the values of c* and A* can be considered constant. For a propellant grain containing a single perforation, the radius of the burning surface will be varying, the equilibrium pressure can still be used as a good approximation for comparing the performance of graded propellant grains with homogeneous counterparts.

Optimal Gradient Architecture

For TSE processed propellants, the burning rate exponent can be assumed nearly constant at 0.4 over the volume fraction range of 0.79 to 0.87, and the propellant density can also be assumed nearly constant. Therefore, the pressure will only vary with the burn rate coefficient, a, and the internal surface area of the cavity, As. It is the desired pressure profile that will determine the resulting gradient architecture. The ratio of maximum to minimum burning rates is typically 1.5. This ratio results in an optimal burning rate profile which is constant until a normalized radius of 0.82, at which point it varies almost linearly to the outer radius (*Figure 7*). If a homogeneous grain is used, the burning rate can not produce a pressure greater than that permitted as the radius of the burning grain approaches the outer radius. Therefore, the grain with the optimal gradient architecture can produce pressures that correspond to a thrust up to 40% greater than that produced by the homogeneous grain (*Figure 8*). The total impulse is directly related to the area under the pressure curves, which is 73% greater for the graded propellant grain. The performance of the graded propellant grains translate into an enhanced payload delivery capability that can more efficiently deliver greater loads at a faster rate over longer distances.

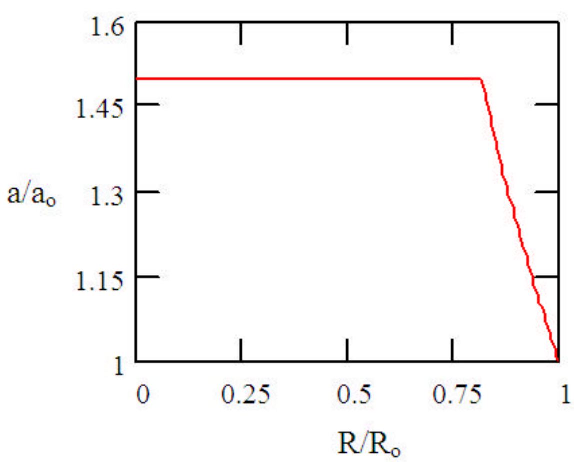

Figure 7. Normalized burn rate profile for optimal gradient architecture that maximizes thrust and total impulse produced by the grain

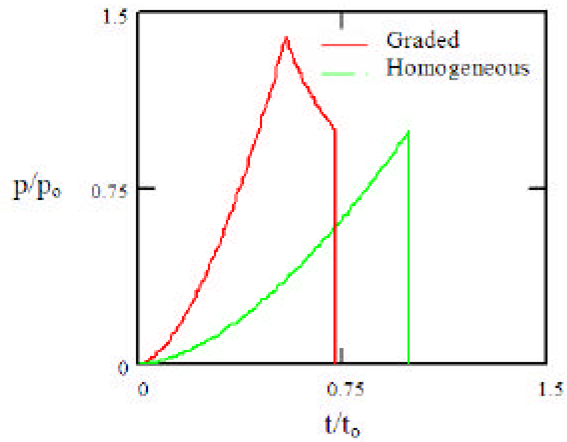

Figure 8. Normalized pressure-time profile for optimal gradient architecture that maximizes the thrust and total impulse produced by the grain compared with profile for homogeneous grain

CONCLUSIONS

Multifunctional energetic structures are being developed using FGM concepts for propellant applications. These materials are being fabricated using Twin Screw Extrusion (TSE) processing, which is capable of producing both axial and radial material gradients. The resulting propellants can exhibit predicted variations in burn rate of 50%. Utilizing a mechanical performance for a pressurized cylinder, the maximum cavity pressure can be predicted for the propellant as a function of the cavity radius. Given a conventional ballistic performance model the corresponding optimal gradient architecture can be determined. The burning rate is nearly constant to a normalized radius of 0.82, at which point it varies almost linearly to the normalized outer radius of 1. For a grain with this optimal gradient architecture, the thrust can be up to 40% greater and the total impulse 73% greater than for a homogeneous grain.

ACKNOWLEDGEMENTS

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