Meso-scale simulation of the configuration-dependent shock-compression response of Ni+Al powder mixtures

D.E. Eakins and N.N. Thadhani *

*Georgia Institute of Technology
771 Ferst Drive NW, Love Building Room 288
Atlanta, GA 30332, USA*

Abstract

Meso-scale simulations of the shock-compression response of nickel and aluminum powder mixtures have been performed to investigate the influence of particle configuration (size, shape, and distribution) on the micromechanical processes of deformation, mass flow, and mixing. Real microstructures were constructed from SEM montages of the starting mixtures pre-pressed at various densities [1]. The travel of the high-pressure disturbance was used to determine the equation-of-state of the mixture material, and compared to the results of real-time experiments for validation. Observations of particle-level processes were used to formulate an understanding of the wide range of macroscopic behaviors exhibited as a function of particle morphology and distribution, porosity, and dissimilarities in properties of the two constituents. The results reveal the effects of particle heterogeneity on the physical, chemical, and micromechanical response of shock-compressed Ni+Al powder mixtures, and their role in the initiation of shock-induced chemical reactions.

Key words: powder consolidation, granular material, deformation inhomogeneities, shock-induced reactions, micromechanical modeling: finite element analysis

1 Introduction

Next-generation materials are being developed with intentionally introduced heterogeneities (spatial variations in physical, mechanical, or chemical state) at various length scales to control their bulk response. As a result, it is becoming more challenging and less accurate to predict the behavior of these

* naresh.thadhani@mse.gatech.edu

next-generation materials from behavior at the bulk-scale. For applications subjected to large strain-rates and dynamic pressures, understanding the influence of meso-scale heterogeneities on the bulk behavior/response of such materials is of paramount importance.

Heterogeneity itself is an ambiguous descriptor, as it can manifest many forms and scales. In shock-compression studies, heterogeneities comprise any local fluctuations in chemistry or structure that act to invalidate the one-dimensional assumptions implicit in the jump conditions used to correlate the states ahead and behind the shock front. Grain boundaries in polycrystalline materials [2], phase boundaries in multicomponent lamellar systems, voids in distended solids, and interfaces and pores in powder compacts, all act as sources from which complex, nonuniform wave structures may emanate. The influence of heterogeneities on the overall shock-compression response depends largely upon the degrees-of-freedom in the system configuration. Powder mixtures are some of the most configurationally-diverse systems; their configuration is defined by parameters such as the number of phases present, size and shape of particles, as well as nearest neighbor and particle orientation distributions.

Over the past several years, it has become increasingly clear that the shock-compression response of powder-based systems is dependent upon their configuration, and cannot be adequately described by equilibrium processes [3]. Shock-compression experiments performed on PTFE powders of 28 μm and 534 μm diameter have yielded a strong correlation between particle size and dispersion of the shock wavefront [4]. For equivalent impact conditions, the front width for the coarse mixture was approximately double the width for the 28 μm powder. The larger particles exhibited longer void-closure times, extending the time required to achieve a steady high-pressure state.

Particle size also plays an important role in the response of energetic powder mixtures. Prior work on the Ti+Si system has revealed evidence of particle-size-dependent dynamic material response [5]. Recovery experiments performed on mixtures of Ti and Si (5:3 molar ratio) of varying particle sizes revealed distinct differences in the particle-level mechanical behavior of the components. For coarse particle sizes (105-149 μm), the Si particles were observed to undergo fracture, fragmentation, and dispersion within the deformed Ti. The mixtures of fine particles (Ti: 1-3 μm , Si: < 10 μm) on the other hand, formed discrete clusters of Ti and Si with limited intermixing. Intermediate particle sizes (< 45 μm) exhibited simultaneous deformation and mixing. These disparate micromechanical behaviors exact direct influence over the propensity for initiating ultra-fast shock-induced chemical reactions, with only the intermediate particle sizes displaying signatures of reaction, evidenced by increases in shock velocity above a threshold stress of 1.5 GPa [5].

Further evidence of the influence of powder configuration on mechanical and chemical behavior has been provided by experimental investigations of Ni+Al mixtures [6]. Recovery experiments performed by Dunbar et. al. on Ni+Al mixtures of varying stoichiometry (3:1, 1:1, and 1:3 molar ratio), particle size (3-150 μm) and particle morphology (equiaxed and flake Ni) showcased different degrees of deformation, mixing, and reaction. It was reasoned that the mixtures of nearly equivolumetric ratios ($3\text{Ni} + \text{Al}$ and $\text{Ni} + \text{Al}$) maximized the probability for simultaneous deformation and mixing, and thereby possessed the greatest potential for reaction. In addition, mixtures containing the flake-shaped Ni particles underwent a unique change in configuration, characterized by ‘smearing’ of the equiaxed Al particles by the harder Ni particles. Likewise, mechanical mixtures of Ni and Al have been shown to exhibit maximum mixing and ability to react under shock compression in contrast to Al coated Ni particles [7].

The significance of these distinct particle-level responses in Ni+Al powder mixtures and their ability (or inability) to react during shock compression was realized following instrumented time-resolved gas-gun impact experiments performed by the authors [8]. Results from experiments conducted up to 6 GPa indicated an inert response for the equiaxed Ni and Al powder mixtures, while the flake-based Ni and equiaxed Al mixture exhibited increased shock-velocities above 3.5 GPa, classically accepted as evidence of shock-induced reaction. These deviations in shock velocity were used to estimate the phases formed during reaction and their extent, however such an analysis is based upon equilibrium thermodynamics, and gives no information concerning the critical particle-level processes responsible for reaction initiation in the short time-scale of the shock pulse duration.

The intent of the work described in this paper is to corroborate the link between configuration change and shock-induced chemical reactions, speculated in prior work on the Ni+Al system [6, 8, 9], through discrete-particle numerical simulations performed on real microstructures of spherical- and flake-based Ni+Al powder mixtures. Principally, this work seeks to address the following questions:

- (1) What is the role of reactant particle configuration, as manifested in the systems explored, on the mechanical response of powder mixtures under shock-compression?
- (2) What particle-scale processes are responsible for shock-induced reaction initiation and product formation?

These questions will be answered following the modeling methods used previously to investigate spherical Ni+Al powder mixtures of various densities [1], and correlated with experimental results documenting the capricious tendency of reaction initiation in the spherical- and flake-based mixtures [8].

2 Background

The limitations of shock-compression experiments in providing the mesoscopic details of deformation and mass flow in porous mixtures have long been recognized. Instrumented experiments employing conventional diagnostics, such as *in-situ* stress gauges and point velocity interferometry, provide temporal resolutions of up to 1 ns, yet are restricted by their poor spatial sampling. While the emergent technique of line VISAR (ORVIS) allows the collection of linearly-resolved data, it remains a surface-sensitive diagnostic. Microstructural characterization of deformation states is only possible as post-mortem observation of the recovered, final state with no information regarding evolution of microstructure or its changes as a function of time.

The particle-scale details of shock-compression in metal powder-based systems is thus, traditionally investigated through computational simulations [10–13]. In many cases, these simulations have relied upon idealized particle geometries and/or distributions. While approximated microstructures may be adequate for systems with highly regular geometries, they are disadvantaged when the powder characteristics are far from ideal, or when the desire is to probe the micromechanics of shock-compression at ever finer scales.

Real microstructures have been used in several cases to simulate the mesoscale deformation and fracture responses of a number of monolithic and composite material systems [14, 15]. The shock-compression response of complex materials has also been studied recently [1, 16]. Benson utilized a pixel-by-pixel correlation technique to import the microstructure of HMX (**h**igh **m**elting-point **e**xplosive) powders into the multi-material Eulerian hydrocode, *Raven* [17]. The simulations examined the local variations in temperature, which matched very well with known mixture theories. The HMX particles used in the study were highly faceted and equiaxed, representing a small excursion from ideality. The accurate prediction of their shock-compression response may not depend as strongly upon the faithful representation of particle geometry as for more irregularly-shaped particles.

The nickel and aluminum powder mixture system studied in the present work is one in which the particles are not as easily characterized by statistical averages and distributions. The particles are of highly irregular geometries, which cannot be easily recreated through the numerical techniques described in previous works [18–20]. The authors have developed an approach to import experimentally acquired SEM montages into the multi-material Eulerian hydrocode, *CTH* [21]. This approach was used to perform discrete-particle numerical simulations on mixtures of equiaxed Ni and Al powders of varying initial density (80-45% TMD). The results were used to better understand the influence of density on the structure and stability of high-pressure disturbance

Fig. 1. Examples of (a) focused flow of grey-contrast Al between dark-contrast Ni, and (b) vortex flow in the 45% TMD spherical Ni+Al simulation. As shown, vortices commonly form within the aluminum flow (with limited Ni), representing poor interparticle mixing.

fronts, and on the dominant particle-level deformation mechanisms [1].

It was also found that the structure of high-pressure fronts in powder mixtures is defined by a low-amplitude elastic-front network, followed by a regime of high-pressure. The elastic-front network comprises the competitive effects of elastic wave propagation through interparticle contacts, and unloading from void pocket regions yet to fully collapse. The network extends ahead of the high-pressure regime by a thickness that depends upon the number of interparticle contacts throughout the mixture. As higher density mixtures contain a greater number of contacts, it follows that the thickness of the elastic-front network increases with density. With decreasing density, the network recedes into the high-amplitude front, carrying with it void pockets of increasing size. The longer closure times associated with the larger voids result in the presence of release pockets within the high-pressure regime. Such pockets serve to create spatial instabilities in pressure, resulting in a highly non-equilibrium state.

The relatively low strength and density of the aluminum particles was responsible for its preferential deformation and the development of two specific flow events. The first, referred to as ‘focused flow’, occurs during the impingement of Al against a restrictive Ni barrier, forcing material at enhanced velocities into the void regions (Figure 1a). The cumulative formation of directionally-varied focused flows into large void spaces had a tendency to evolve into the second flow event, known as ‘vortex formation’ (Figure 1b). While these were regions of enhanced flow and high temperature generation, the vortices consisted almost exclusively of Al, and did little to deform and incorporate any neighboring Ni.

3 The Ni+Al System

The Ni+Al powder mixture is an example of a system with large intrinsic heterogeneity. The physical and mechanical properties of the components are highly dissimilar; density, yield strength, and shear modulus all differ by over 200%. Such differences are responsible for the preferential deformation and limited mixing of the softer Al phase with the harder Ni. It is unsurprising then, that the equiaxed Ni+Al powder mixture system exhibits difficulty in reacting through shock-induced mechanisms at low pressures (< 6 GPa) [22].

Though challenging to react, the formation of the equiatomic *NiAl* phase results in a high heat of reaction, $\Delta H = -1.38$ kJ/g. Indeed, recovery experiments reveal that intermetallic reactions initiated through thermochemical mechanisms are sufficiently exothermic to melt the immediate product phase [6, 23]. Such exothermic potential, with the ability for rapid release of energy, is desired for next-generation energetic materials. These new materials need not only to deliver a certain energetic output, but also within a flexible timescale. For low reaction-threshold materials, this requires methods for controlling sensitization. Conversely, techniques may be investigated for increasing the susceptibility to ultra-fast reactions in the high reaction-threshold Ni+Al system. The advantage of the latter approach is in applying the understanding gained through this work to the large matrix of intermetallic-forming systems, effectively increasing the number of candidate systems with widely varied differences in reactant properties for next-generation energetic materials.

The objective of this work is to use starting powder configuration (e.g., particle morphology and/or packing density) as a design parameter, through which the desired energetic response of shock-induced chemical reactions may be promoted, in spite of the intrinsically heterogeneous but highly exothermic Ni+Al powder mixture system.

4 Model Description

The simulations of shock compression were performed using the multi-material Eulerian hydrodynamic code, CTH, developed at Sandia National Laboratories [21]. The powder microstructures were constructed from real micrographs obtained from pre-pressed Ni+Al powder mixtures of varying density (80%, 60%, 52%, and 45% TMD) and configuration (spherical and flake particle morphologies). The various configurations of powder mixtures were pressed to the desired initial density, and then sectioned along the pressing axis. A fraction (slightly less than the desired void volume fraction) of *Loctite Hysol*

Fig. 2. Scanning electron micrographs and imported CTH model domains for the 45% TMD spherical Ni+Al, and flake Ni + spherical Al powder mixtures. The Ni particles in the flake mixture form layered stacks normal to the pressing direction (vertical).

epoxy was added before pressing to facilitate sectioning and polishing of the highly-porous compacts. The source SEM montages and resulting CTH model domains for the 45% TMD spherical Ni+Al and flake Ni + spherical Al powder mixtures are shown in Figure 2. The procedure used to transfer the real particle shapes into the model environment are described elsewhere [1].

The model domain spanned 1.62 mm in height, and 0.261 mm in width. Periodic boundaries were prescribed at the left and right edges to approximate

an infinite medium, while material was permitted to enter and exit through the upper and lower edges. Several mesh sizes were employed, depending upon the powder microstructure. A flat resolution of $1\text{ }\mu\text{m}$ per cell edge was used in the case of the spherical Ni+Al mixture, while three resolutions, coarse ($1\text{ }\mu\text{m}/\text{cell edge}$), medium ($0.5\text{ }\mu\text{m}/\text{cell edge}$), and fine ($0.25\text{ }\mu\text{m}/\text{cell edge}$) were used for the flake Ni + spherical Al configuration. The hydrodynamic mechanical response of the nickel and aluminum components was described by a Mie-Grüneisen equation-of-state, while the strength was governed by the Steinberg-Guinan viscoplastic model for high strain-rates [24]. The shock was delivered by the motion of a copper piston from the lower edge, at particle velocities of 0.5, 0.75, and 1 km/s.

5 Results

An in-depth multiscale characterization of the influence of particle morphology on the shock-compression response of Ni+Al powder mixtures was accomplished. In as much as possible, observations are made between mixtures of equivalent density (45% TMD), but different Ni morphology. First, validation of the simulations based upon comparisons to experimental $U_s - U_p$ data are presented. The structure and stability of the high-pressure fronts in the spherical and flake-shaped powder mixtures are then compared. Next, the spatial and temporal dispersion of the advancing peak stress front are measured across the sample width. The heterogeneity of pressure and temperature following void collapse are also noted. Finally, the complex mechanisms of deformation and their evolutions, specific to each component and powder mixture configuration, are characterized from sequences of images captured at different times. Through comparisons between the simulations performed on the micron-scale spherical and flake-shaped Ni+Al mixtures, mechanisms leading to and responsible for the initiation of shock-induced chemical reaction are proposed.

5.1 Bulk-level Validation

The numerical simulations of the shock-compression of Ni+Al powder mixtures were validated at the macro-scale on the basis of equation-of-state. The simulated equation-of-state of each mixture was determined by correlating the particle velocity, U_p (assigned to the Cu driver), with the resulting shock velocity, U_s . The shock velocity was obtained by noting the arrival-time of the peak amplitude front after propagation distances of 1.0 and 1.5 mm for the spherical mixture, and 0.4, 0.8, 1.0 and 1.5 mm for the flake mixture.

The simulated $U_s - U_p$ fits were compared to data obtained from time-resolved plate-impact experiments performed in previous studies [8, 9, 22]. In these experiments, a nearly one-dimensional supported shock pulse was used to dynamically compress a thin (<3 mm thick, 50.8 mm in diameter) layer of nickel and aluminum powder mixture. *In situ* PVDF stress gauges located on either side of the powder layer provided measurement of the amplitude of the shock pulse entering and exiting the specimen, and of the shock velocity, determined by the time of travel through the mixture thickness. Through use of the Rankine-Hugoniot relations, the $U_s - U_p$ equation-of-state of the specimen was determined.

Figure 3 shows the $U_s - U_p$ data obtained through experiments and simulations for the 60% TMD spherical Ni+Al, and 45% TMD flake Ni + spherical Al powder mixtures. The error bars on the experimental data points correspond to uncertainties in powder density, thickness, and shock transit time, while those for the simulation results (indicated by the narrow band) originate from the uncertainty in locating the position of an irregular shock front. The simulation closely matches the experimental data for the 60% TMD specimen. In the case of the 45% TMD mixture, the simulation only fits the lower end of the experimental data, albeit offset to lower shock velocities. This offset is ascribed to the 2-dimensional symmetry of the model, and the omittance of out-of-plane particles and contacts that would otherwise assist in the progression of the shock front. The upper portion of data contains the signature of shock-induced chemical reaction, discussed elsewhere [8], which is not reproduced by the current model; the model only simulates the evolution of mechanical configuration, and does not consider changes in chemistry. Regardless, the mechanisms responsible for the initiation of ultra-fast chemical reactions can be revealed by investigating the principle differences between the shock response of the spherical- and flake-based powder mixtures at the front and particle level.

5.2 Front character

The structure and stability of high-amplitude pressure fronts through equiaxed granular materials has been shown previously to be dependent upon the initial density and particle velocity. The influence of powder configuration is investigated by comparing pressure surfaces constructed in the spherical and flake models of equivalent initial density (45% TMD) at $U_p = 1$ km/s. Figure 4a shows the pressure surface for the spherical Ni+Al mixture. The surface consists of a leading front, followed by a region of high-amplitude pressure. The front spans a thickness of nearly $100 \mu\text{m}$, its irregularity caused by competition between rapid loading of particles and unloading from voids that have yet to collapse (release pockets).

Fig. 3. Comparison between measured and simulated $U_s - U_p$ data for the 60% TMD spherical Ni+Al, and 45% TMD flake Ni + spherical Al mixtures. Note, the simulation does not predict the increased shock velocities in the flake mixture at higher pressures, due to omitted details of chemical reaction.

A similar characterization was also performed for the shock front in the flake Ni + spherical Al powder mixture. Shown in Figure 4b is the pressure surface constructed after a shock transit time of 250 ns for the fine mesh model. Note the narrow thickness of the elastic front network, which is on the order of tens of microns (10-40 μm). This thickness is consistent with the results of the 45% spherical Ni+Al mixture, and is attributed to the small number of interparticle contacts at the low density. The rise of the high-amplitude portion of the surface spans an even smaller distance, and is followed by a seemingly constant regime of pressure. These observations are in stark contrast to the trend witnessed in the spherical mixture, i.e., shocked-state stability decreases with mixture density. The numerous release pockets within and immediately following the front in the 45% TMD spherical mixture are entirely absent; the front not only appears to be stable, but highly planar. The absence of the release pockets is attributed to the configuration of the void spaces within the microstructure. Unlike the void spaces in the spherical mixture, which form a large (at least a particle diameter in size) nearly contiguous network, the void within the flake mixture is evenly distributed between the stacked flakes. Thus, the void regions, while likely to be contiguous, are never more than a few flake dimensions thick (~ 600 nm). This results in a very rapid closure of the void space which, combined with the even distribution and packing of the particles throughout the thickness of the specimen, yields a highly planar, nearly stable high-amplitude stress front.

Another indication of the stability of these high-amplitude stress fronts can be seen in Figure 5, which is a comparison between the pressure profiles constructed for the spherical and flake Ni+Al mixtures. For the equiaxed mixture, the profile contains several dips (indicated by the arrows), which are the signature of release from the void spaces. These dips serve to stretch the front,

Fig. 4. Pressure surfaces in the spatial domain constructed for the 45% TMD (a) spherical Ni+Al, and (b) flake Ni + spherical Al simulations. Note the narrow width and planarity of the shock front in the mixture containing flake particles relative to the spherical mixture.

Fig. 5. Comparison between the pressure profiles of the (a) spherical Ni+Al, and (b) flake Ni + spherical Al mixtures. The rise time of the spherical mixture is approximately 74 ns due to the influence of release pockets (arrows), whereas it is only 15 ns for the flake mixture, caused by the even distribution of void space.

extending the time required to achieve the high-amplitude state (rise-time) to approximately 74 ns. This time is considerably longer than that for the flake mixture, which is approximately only 15 ns. Such broadening of the shock front is commonly referred to as ‘dispersion’, and is frequently observed in the time-resolved records obtained from porous materials [4, 25–27]. In addition, the pressure following the rise to peak amplitude is also sensitive to particle morphology, varying by only ± 1 GPa for the flake mixture, as compared to ± 2 GPa for the spherical powders. Pressure variations of the magnitude shown following the shock front are not detected by experimental measurements, which instead obtain an averaged measure of material response. It should be noted that these characteristics of the high-amplitude front are representative of profiles obtained at several locations throughout the spherical- and flake-based Ni+Al mixture models. In the equiaxed mixture, such front character does not meet the definition of a stable shock. Only the flake mixture, with its narrow front width, stable high-pressure state, and quasi-planar structure,

appears to develop a true shock front.

Next, the influence of powder configuration on thermo/mechanical response at the front-level was investigated through field plots taken at the various particle velocities simulated. Figure 6 shows the local cell pressures and temperatures for the spherical and flake mixtures from 260 μm fields near the high-amplitude front, presented according to particle velocity (0.5, 0.75, and 1 km/s). Cell temperatures were calculated from the contributions of PdV mechanical work and artificial viscosity. At $U_p = 0.5$ km/s, the cell pressure and temperature fields appear to be quite homogeneous for both configurations. The only noticeable variations are observed in the increased temperature at the aluminum particle peripheries, and are on the order of only a few hundred degrees. As the particle velocity is increased, the cell pressures throughout the field become progressively more spread, the greater effect being observed in the spherical mixture ($\Delta P > 10$ GPa). The pressure spikes in the flake mixture are isolated and few, caused by impinging of adjacent aluminum particles. Generally, the pressures in the flake mixture at $U_p = 1$ km/s range from $\sim 3\text{--}5$ GPa. The changes in temperature with particle velocity are less mild. In the spherical mixture, substantial heating (> 1200 K) is produced within the flow channels of aluminum, while the nickel particle interiors remain largely undisturbed. On the other hand, the reverse is true for the flake mixture, in which the cells containing nickel and the aluminum particle exteriors experience significant increase in temperature (> 1200 K), while the aluminum interiors see a marginal change. Perhaps most significant is the difference in the localization of temperature between the two configurations. While in the equiaxed mixture the heat is highly concentrated within the discrete flow channels, the increased temperature in the flake mixture appears to be more evenly distributed throughout the nickel flakes. It should be noted that while it is possible to measure “bulk” shock pressures using stress gauges, the measurements provide a response averaged over the area spanning the gauge and corresponding sample thickness. Measurements of stresses and temperatures evolving at the local particle scale are not possible, which makes it difficult to validate the response illustrated in Figure 6. Nevertheless, the simulations shown supply important information regarding differences in the local thermomechanical response, as a result of powder configuration.

5.3 Scatter Diagrams

The pressure line plots and field diagrams are useful for illustrating the spatial or temporal distribution of pressure and temperature. In some cases, it is also desirable to view the correlation between several different variables, and thus characterize the state of the compressed region. The pressure-volume states derived from the experimental results are an example of a correlated

Fig. 6. Pressure and temperature fields as a function of both particle velocity and morphology. A greater spatial variability in state is observed in the spherical mixture, evidenced by the highly localized pressures at particle point contacts, and temperatures within discrete flow bands.

plot between load and strain. As described in the previous sections however, the experimental measurements supply averages of local behavior, and consequently are insensitive to local fluctuations and instabilities. For this reason, a unique diagram was developed that would both correlate several perceived important state variables, and preserve the inhomogeneous nature of the compressed zone.

The diagrams that were constructed are three-variable scatter plots, two of the variables of which are pressure and strain. The third variable is known as the *nearest reactive neighbor distance* (NRND), and is the minimum distance separating cells containing reactive partner species. The first two variables were supplied directly from the CTH database, while the third was calculated in a data post-processing step. The intent of these diagrams was to reveal the distribution in states achieved during the consolidation process, and in particular, the evolution of the distance separating reactive neighbors. The data for the scatter diagrams was taken from a fixed Eulerian window that encompassed the entire model width, and spanned $199.8 \mu\text{m}$ for the spherical mixture, and $204.5 \mu\text{m}$ for the flake mixture. Diagrams were constructed at intervals of 5 ns, starting from the time when the shock front entered the window, up to the time when the front had passed entirely beyond the upper window boundary.

Fig. 7. Scatter plot for the 45% TMD spherical Ni+Al powder mixture constructed from a fixed Eulerian window after 100 ns. The states from both components are widely scattered, exhibiting large variations in pressure and strain. The aluminum states appear to show slightly higher levels of strain, when compared to the nickel states.

Scatter diagrams constructed 100 ns after the arrival of the shock front are shown for the spherical and flake Ni+Al powder mixtures in Figures 7 and 8, respectively. The diagrams for both components share the same strain and NRND axes, while the pressure axis is discontinuous. For the spherical mixture, both components exhibit a wide scatter in strain, pressure, and NRND. The bulk of the pressures (ignoring upper-end scatter) span nearly the same range for both components, $\sim 0 - 8$ GPa. The spread in strain, on the other hand, is larger for aluminum than nickel. The maximum strain in aluminum is approximately 10-12, while for nickel it is only 5. The nearest reactive neighbor distances also see a large variation, and range from 0 (in contact) to $> 15\mu\text{m}$. It is not surprising to see such large ranges, as the line profiles and field diagrams also indicated a highly heterogeneous macro-scale and local response. Also, it would appear from the equivalent range in NRND between components, that there remain large particle interiors for both nickel and aluminum that are removed from their reactive partners by tens of microns.

The pressure, strain, NRND scatter diagram constructed after 100 ns for the flake mixture exhibits a markedly different appearance. The states for both the nickel and aluminum components have a dramatically reduced spread in pressure (± 1 GPa), suggesting that a nearly equilibrium mechanical state is achieved. Furthermore, the maximum strain in the aluminum is about 6, while

Fig. 8. Scatter plot for the 45% TMD flake Ni + spherical Al powder mixture constructed from a fixed Eulerian window after 100 ns. Both the nickel and aluminum states have a very narrow spread in pressure, suggesting a rapidly achieved mechanical equilibrium. The NRND of the aluminum is greatly reduced to approximately 5 μm . Like the spherical mixture, the aluminum particles occupy a larger distribution of strain that the nickel particles.

that for nickel 4. Thus, the difference between the maximum strains in either component is reduced ($\Delta\varepsilon_{max} = 2$ for the flake mixture versus 5-7 for the spherical mixture). The change in NRND is also quite significant. The distance separating the deformed aluminum particles is concentrated heavily within the 0 – 5 μm range, while the distance for the nickel particles is between 0 – 17 μm . These results indicate that the configuration of the aluminum particles is changing in such a way as to reduce the distance between their interiors and nickel. Nickel, on the other hand, retains regions very well removed from aluminum, which is evidence of the development of clusters. It should be noted, however, that these measures are determined from 2-dimensional models, the reduced dimensionality has the largest impact on the nickel flake NRNDs. Since the flattened aluminum particles are almost exclusively bordered in-plane by nickel, little change is expected from considering out-of-plane nickel flakes. The nickel flakes, on the other hand, are highly clustered in-plane, the nearest aluminum particle commonly removed by tens of flake thicknesses. An out-of-plane aluminum particle could have a significant impact on the NRND.

Further interpretation of these plots requires a meso-scale characterization of deformation at the particle level.

Fig. 9. Series of images showing the flattening of aluminum particles at the shock front in the flake mixture. Total time is 45 ns, corresponding to a local particle strain rate of $5e^9$.

5.4 Deformation Mechanisms

As discussed in prior work [1], the primary particle-level responses in the equiaxed mixtures are preferential deformation of aluminum, focused flow, and vortex formation. The micro-mechanical features of particle deformation differ greatly between the spherical and flake Ni+Al powder mixtures. While the aluminum particles in the spherical mixture experience preferential deformation and mass flow over large distances, those in the flake mixture undergo a very unique change in configuration during shock compression. Shown in Figure 9 is a series of snapshots from the fine scale flake Ni + spherical Al mixture model that follow the ‘flattening’ of two nearly spherical aluminum particles. Such flattening is the cumulative response of the particles first impinging against the compressed zone, and then subsequently colliding with the nickel flakes that immediately follow. Massive aluminum flows are not formed simply due to the lack of large, open, void space. The homogeneous distribution of nickel flakes (and thus, void space) guarantees that most aluminum particles are separated from one another by layers of nickel flakes. This configuration leads to severely flattened aluminum particles of highly increased surface area.

The processes of focused flow and vortex formation still occur in the flake mixture, although due to different mechanisms. Since the layered nickel flakes obstruct flow in the direction of shock propagation, most focused flow occurs laterally. The formation of such a focused flow leading to a lateral vortex is isolated in Figure 10. As shown through the sequence of images, a focused flow of aluminum is forced into an adjacent aluminum particle. After 5 ns, a vortex begins to take shape at the impingement site. Unlike the vortices in the spherical mixture, these lateral vortices can easily draw in particulates of nickel, due to the fine structure of the flakes.

Fig. 10. Lateral vortex in the flake Ni + spherical Al mixture. The Ni flakes are easily incorporated into the flow, due to their fine structure.

5.5 End-state Configuration

The significance of the local deformation processes observed in the spherical and flake-shaped powder mixtures, in terms of their affect on reaction susceptibility, can be inferred from simulated micrographs of the final, consolidated powder configurations, shown in Figure 11. End-states are shown for the (a) 60% and (b) 45% TMD spherical Ni+Al mixtures, and (c) 45% flake Ni + spherical Al mixture, following simulation at $U_p = 0.75$ km/s. The 60% spherical mixture clearly exhibits preferential deformation of Al (dark grey), evidenced by the large, relatively undeformed clusters of Ni (light grey). At 45% TMD, the aluminum flows have grown in size and turbulence, imparting a greater degree of damage to the Ni particles. Notice that the deformation history is quite evident in the remnant flow patterns, and that the evolved mixture configuration is highly heterogeneous; regions of varying degrees of mass flow and particulation exist in the microstructure. In contrast, the end-state configuration of the flake Ni+Al mixture is far more homogeneous, with evidence of lateral flow during the flattening process observed for every Al particle.

As reaction initiation must occur at the interfaces between Ni and Al, an indirect measure of the potential for wide-scale reaction may be obtained from the amount of intimate surface contact in the microstructure. Line-intersection analysis was performed on the simulated end-state microstructures of the spherical powder mixtures of varying density, and the 45% TMD flake mixture, to estimate the Ni/Al interface area per unit volume, S_V [28] as a function of initial particle velocity. As shown in Figures 11 and 12, the amount of Ni/Al interface area in the spherical mixture increases with increasing porosity (decreasing %TMD) and particle velocity. The 45% TMD spherical mixture exhibits the largest increase in Ni/Al interface at $U_p = 1$ km/s. This increase reflects the enhanced deformation and particulation caused by the increased void volume and extended void closure times. When the morphology of the

Fig. 11. Final, end-state micrographs simulated ($U_p = 0.75$ km/s) for the (a) 60% TMD spherical Ni+Al, (b) 45% TMD spherical Ni+Al, and (c) 45% TMD flake Ni + spherical Al mixtures, and the associated nickel/aluminum interface area per unit volume, S_V . The amount of intimate interface in the flake mixture is greater than that for both spherical mixtures, revealing a tremendous change in configuration.

Fig. 12. Plot of interface area per unit volume, S_V as a function of particle velocity for the 80%, 60%, and 45% TMD spherical mixtures, and the 45% TMD flake mixture.

Ni particles is changed from spherical to flake, an even greater increase in the amount of Ni/Al interface area is observed (nearly doubled at $U_p = 0.5$ km/s, at an equivalent density). A similar analysis performed on a 60% TMD spherical Ni+Al specimen recovered following an impact experiment at $U_p = 0.55$ km/s yielded a measure of $S_V = 99.1 \text{ mm}^{-1}$, and is also shown in Figure 12. This is nearly identical to the simulated value of 101.3 mm^{-1} at $U_p = 0.5$ km/s for the same powder configuration, validating the deformation and flow behavior of the constituents within the regime compared.

6 Discussion

6.1 Particle-level Deformation Processes

The simulations of the shock-compression of Ni+Al powder mixtures have provided evidence of morphology-dependent behavior across several scales. These differences observed at the front-level, clearly show that particle morphology directly affects the planarity, stability, and rise-time of the high-pressure disturbance. The shock-like structure of the disturbance in the flake mixture is at the very least an indication that local deformation processes are distributed homogeneously behind the front.

At the particle level, it becomes clear that the specific make-up of the particles bordering the void spaces has a large effect on the precise mechanical and thermochemical states evolved. As the powders considered in the present work are far from ideal, they can take up a limitless number of elaborate configurations. These configurations simply add to the complexity of particle deformation and intermixing. The simulations showed that mechanisms such as focused flow, particulation, and vortex formation were active in the micron-scale spherical Ni+Al powder mixtures, and are fundamentally linked to the preferential deformation of aluminum and annihilation of the void space. The large contiguous void volume in the spherical mixture permits the aluminum flow to grow in turbulence, and dictate deformation in adjacent regions. According to Graham [29], ‘mixing will be expected whenever local heterogeneous deformation is encountered’. From the current work it is clear that while the above statement is true, *extensive* mixing is not necessarily guaranteed. In the spherical mixture, aluminum vortexes appear to draw in very little nickel from adjacent particles and clusters. As shown in Figure 1b, vortex motion near a nickel particle does not accomplish any breakup or incorporation of the neighboring nickel. These regions serve instead as sources of increased temperature, which can evolve into thermochemical initiation sites, albeit at extended time scales (tens of microseconds or later). Such evidence of reaction products ($NiAl_3$) within regions of vortex flow has been observed in the recovered micrographs of a spherical Ni+Al mixture shock-compressed at 998 m/s [22].

The simulations performed on the flake Ni + spherical Al mixture yielded quite different deformation characteristics. As discussed above, the distribution of flakes and void space results in a highly planar, rapidly equilibrated high-amplitude front. It also follows that the configuration of the flakes serves to isolate the aluminum particles from one another. Thus, as the particles are shock-compressed, focused flow can only occur laterally, and into a void space far more limited in size than the contiguous networks in the spherical

mixture. As a result, the spherical particles are swiftly brought into mechanical equilibrium, as seen in the scatter diagrams, and deformation cascades are eliminated. This serves to keep the front planar, and devoid of release pockets. An indication of the degree of flattening that occurs ($U_p = 1$ km/s) can be obtained from the evolution of nearest reactive neighbor distance. After 80 ns, the maximum mean NRND for aluminum is approximately $5\text{ }\mu\text{m}$. This is reduced from a starting maximum distance of $17\text{ }\mu\text{m}$. On the other hand, the NRND for nickel remains undiminished ($17\text{ }\mu\text{m}$). This large disparity between mass transport distances suggests that reaction will be only localized around the aluminum particles.

6.2 Chemical Reaction Mechanism

From the observations of shock-compression behavior of reactive powder mixtures at several scales, we can begin to formulate an explanation for the varied deformation and consequent chemical response of the spherical and flake Ni+Al powder mixture systems. The difficulty in initiating shock-induced reactions at the high-pressure state in mixtures of Ni and Al powders of spherical morphology appears to be due to a combination of the preferentialism of deformation, and the large consolidated void spaces. The bulk compression is highly partitioned between the two components, which produces a highly activated (strained) aluminum matrix surrounding large, relatively undisturbed nickel clusters. Vortexes are frequently observed within the aluminum flow, yet these contain very little nickel for mass mixing. While shock-induced reaction may be initiated in select regions, the widely varying states of temperature, deformation, and mixing throughout the compressed zone make it unseemly that such reaction pockets will be sustained over longer times, and thereby influence the measured macroscopic shock-compression response.

In contrast, all of the Al particles in the flake powder mixture system appear to become severely flattened by the advancing wave front. This phenomenon is reflected by the highly stable high-pressure state and low NRND for aluminum. As the aluminum is flattened from a sphere into an oblate spheroid, the surface area in contact with nickel increases. This can be shown by approximating the aluminum particles as perfect spheres, and calculating the relative surface area as a function of spheroid eccentricity. By respectively assuming an original radius and final minor radius of $17\text{ }\mu\text{m}$ and $5\text{ }\mu\text{m}$, the dissimilar particle surface contact area is increased by approximately 80%. Furthermore, line intersection measurements revealed a significant increase in the Ni/Al interface area in the flake mixture relative to the spherical mixture. This large increase in interface area results in the exposing of nascent, fresh reactants. Previous researchers have identified this mechanism as one of several critical processes for the initiation of chemical reactions [30]. It is

hypothesized that each and every aluminum particle acts as a reaction initiation site, with mixing facilitated by the shear produced during the rapid lateral flow of the compressed aluminum particle. The fine structure of the nickel flakes further promotes mixing, by more easily being drawn into the lateral flows and vortexes with aluminum. Such processes are consistent with the observations made by Horie, who has pointed to Helmholtz instabilities, microjetting, and dispersion of material within vortexes as necessary mixing mechanisms for reaction [31,32]. The interparticle shear produced during flattening and lateral flow of the aluminum particles in the flake mixture is also similar to the mechanics described by Dremine’s *ROLLER* model [33]. During flattening, new material is progressively fed into the interface. The sliding interface between nascent aluminum and fine-structured nickel may initiate reaction through such a mechanism. In short, the propensity for the flake mixture to react is due solely to the creation of Al/Ni boundaries, through transport of nascent, aluminum particle interiors into nickel at the interparticle boundaries during the flattening process. To explore this effect in more detail, molecular dynamics or atomistic simulations need to be conducted to investigate how the dissimilar atoms are drawn into the reaction zone, and lead to reaction product formation.

These results do well to address the questions posed earlier concerning the influence of configuration on the mechanical and shock-induced chemical response of powder mixtures. Additionally, they can be used to elaborate upon the details of the *CONMAH* schema, a conceptual model proposed by Graham to describe the general processes (**configuration** change, **mixing**, shock **activation**, and **heating**) leading to shock-induced chemical reactions [34]. Figure 13 shows the *CONMAH* model updated with the results of the discrete particle simulations. In this schematic, material in the original configuration (shown at left) is brought to a final, compressed configuration (shown at right) through the transition zone. Prior to this work, the particular events within the transition zone were speculated [33, 35, 36], but unknown. The current simulations reveal that the character of the transition zone depends strongly on the initial configuration, which leads to variations in the structure (dispersion, irregularity) and stability (release pockets) of the shock-wave front, and particle-level deformation and mixing behavior. The combined interpretation of experiments and simulations suggests that shock-induced chemical reactions are initiated more easily in systems with a narrow, abrupt transition zone, symbolic of the quasi-homogeneous distribution of porosity and local deformation response.

The elaborated *CONMAH* model summarizes the shock-compression response of both equiaxed- and flake-shaped Ni+Al powder mixtures illustrating reasons for the lack of (in the case of the former) and/or the cause of (in the case of the latter) shock-induced reactions in these systems. As such, the transition zone and particle-level features shown are particular to the systems investi-

Fig. 13. Schematic illustrating the updated *CONMAH* model with details of the transition zone and possible processes influencing configurational changes supplied by the current investigation.

gated, and are not expected to be applicable to all classes of material systems. Other material combinations, e.g., ceramic + metal, polymer + metal powder mixtures, may exhibit differing modes of deformation, fracture, dispersion, and mixing, possibly reaching its reacted configuration through a different transition zone. Similar experiments and computations must be completed on these systems in order to establish a more global understanding of the transition zone, and its role in shock-induced chemical reactions.

6.3 Limitations and Considerations

The simulations shown represent the first computational study of the shock-compression of multi-component powders employing real, imported microstructures. This approach is necessary to describe the particle-level processes that are not captured through real-time experimental diagnostics. However, it should be noted that there are several limitations and caveats to the present work. The first concern is the level of validation that currently exists between ex-

perimental work and discrete-particle simulations. As shown in this work, validation exists at the bulk scale ($U_s - U_p$, EOS fitting), the front scale (rise-time observations), and at the end-state (measure of S_V). On the other hand, there is no method of experimentally obtaining the necessary data needed to validate the local responses simulated in the current work. As yet, there is a disparity between the length-scales respectively sampled or represented in experiments and simulations. This lack of data at the particle-level makes validating the appropriateness of the material strength models, and resulting transient deformation modes and structures, difficult. In defense of the current work, however, it should be reminded that very good agreement exists in the validation of the end-states (Figure 11). It should be realized that the end-state is very much path-dependent, and that such agreement cannot be achieved if the transient behavior is simulated incorrectly. This argument is, of course, entirely speculative, and will have to suffice until better techniques are developed to validate the processes at the particle-level.

The second limitation of the current work lies in the 2-dimensional representation of a 3-dimensional problem. Certainly, it is acknowledged that the heterogeneity of powder mixtures extends in every dimension, and that the omittance of the third dimension removes z -displacements and xz , yz rotational modes. In addition, any out-of-plane features (particles, voids) that affect in-plane behavior are also ignored. Such reduced dimensionality will have varying degrees of influence from specimen to specimen. In mixture configurations where out-of-plane flow is minimized, the inaccuracies arising from a 2-dimensional model are lessened. This is the case for the higher density spherical mixtures and flake mixture, where the small contiguous void spaces led to rapid void collapse. Efforts to import real microstructures in 3-dimensions is already well underway, and is being accomplished through the technique of serial-sectioning. Future studies on these 3D models will lead to a more quantitative evaluation of the importance of reduced dimensionality.

7 Conclusions

Discrete-particle numerical simulations of the “shock”-compression of real, imported microstructures was performed in order to determine the link between particle morphology and experimentally-observed shock-induced reactions in Ni+Al powder mixtures. Results indicated that particle morphology has significant influence over the structure and stability of disturbance fronts, and the micromechanics of particle deformation. The difficulty in initiating ultra-fast reactions in the spherical mixture at modest pressures is caused by a combination of large, contiguous void spaces, and hard, equiaxed Ni particles. The net result is the cumulative preferential deformation of many softer aluminum particles into the void regions, limiting the degree of interparticle mixing.

In contrast, stacking of the Ni-flakes in the flake mixture resulted in the homogeneous distribution of the void space; the size of the voids was on the order of several flake thicknesses. This configuration led to rapid flattening of the aluminum particles, and doubling of the particle surface area. The trapping of aluminum by the flakes prevented the build-up of deformation cascades, and forced all deformation to be localized. Vortexes produced through lateral flow were observed to incorporate significant nickel, due to the fine structure of the flakes.

These results provide further evidence of the influence of configuration on the mechanical and chemical response of intermetallic-forming powder mixtures. Understanding the details of configuration change within the transition zone is an essential step to controlling the shock-response of heterogeneous materials. Extending this understanding throughout the gamut of heterogeneity will ultimately provide the ability to synthesize new materials with predefined behavior, and allow control of reaction and associated energy release for energetic material applications.

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