

## CHARACTERISTICS OF SHOCK-COMPRESSED CONFIGURATION OF Ti AND Si POWDER MIXTURES

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Shock-compression recovery experiments were performed on mixtures of Ti and Si powders of **fine**, **medium**, and **coarse** morphology, and packed at different initial densities, using the Sandia Momma and Poppa Bear fixtures with Baratol explosive. The shock-compressed configuration revealed characteristics typical of either chemically reacted material with **fine** equiaxed grains, or unreacted material with densely packed Ti and Si particles. The unreacted configuration showed that Ti particles were extensively deformed, irrespective of powder morphology and shock conditions generated by either fixture. In contrast Si particles showed different characteristics depending on the powder morphology, packing density, and shock conditions. The microstructural characteristics of unreacted configuration of Ti and Si powder mixtures were investigated. Mechanistic processes occurring prior to the inception of *shock-induced chemical reactions* in this system are described.

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## INTRODUCTION

Titanium-silicon represents an highly exothermic intermetallic forming system, with associated heat of reaction of -138kcal/mole, volume change of -27.8%, and calculated reaction temperature of 2500K for the formation of  $Ti_3Si_3$ .<sup>1</sup> Shock-compression experiments<sup>2</sup> on Ti-Si powder mixtures have shown that chemical reactions in this system occur at shock pressures of only a few GPa, and corresponding bulk temperatures significantly below the melt temperature of Si. The equilibrium shock temperature (and shock energy) does not influence the reaction behavior. Rather, by altering the shock pressure and initial packing density, but maintaining the same bulk temperature, it is found that the propensity for reaction initiation largely depends on particle size, with **fine** powder morphologies reacting at lower pressures and lower initial porosities<sup>2</sup>.

The objective of our present work is to study this system in detail via controlled instrumented and recovery experiments on the same types of powder mixtures and under similar loading conditions. The results of real-time measurements are discussed by Dunbar et al<sup>3</sup> in this proceedings. Results of recovery experiments focussing on characteristics of shock-compressed unreacted configuration of Ti-Si powder mixtures at conditions below the reaction threshold, will be described here.

## EXPERIMENTAL PROCEDURE

Shock recovery experiments were performed on Ti-Si powder mixtures of three types of powder morphologies, **coarse** (105-149  $\mu m$  Ti and 45-149  $\mu m$  Si), **medium** (10-45  $\mu m$  Ti and Si), and **fine** (1-3  $\mu m$  Ti and < 5  $\mu m$  Si). The powders were mixed in a mortar and pestle (without organic mixing agents) in a volumetric distribution corresponding to the  $Ti_3Si_3$  atomic stoichiometry compound. SEM images of the respective powder mixtures are shown in Fig. 1.

The various powder mixtures were shock loaded using the Sandia<sup>4</sup> Poppa Bear fixture with Baratol explosive (PB-B) and Momma Bear fixture with Baratol explosive (MB-B). In these fixtures the loading history is dominated by an initial low-pressure planar wave, followed by a radial wave focussing effect, resulting in peak pressures of  $5 \pm 1$  GPa for PB-B system and  $7.5 \pm 2.5$  GPa for MB-B system.<sup>4</sup>

Six experiments were performed on powder mixtures of **medium** morphology packed at initial density ranging between 53% to 64% (or porosity of 47% to 36%) with MB-B fixture, and 45% to 53% (or porosity of 55% to 47%) with PB-B fixture. Two experiments were performed on **fine** and **coarse** morphology powders, each with packing density of 64% (36% porosity) with MB-B, and 53% (47% porosity) with PB-B fixture.

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## **DISCLAIMER**

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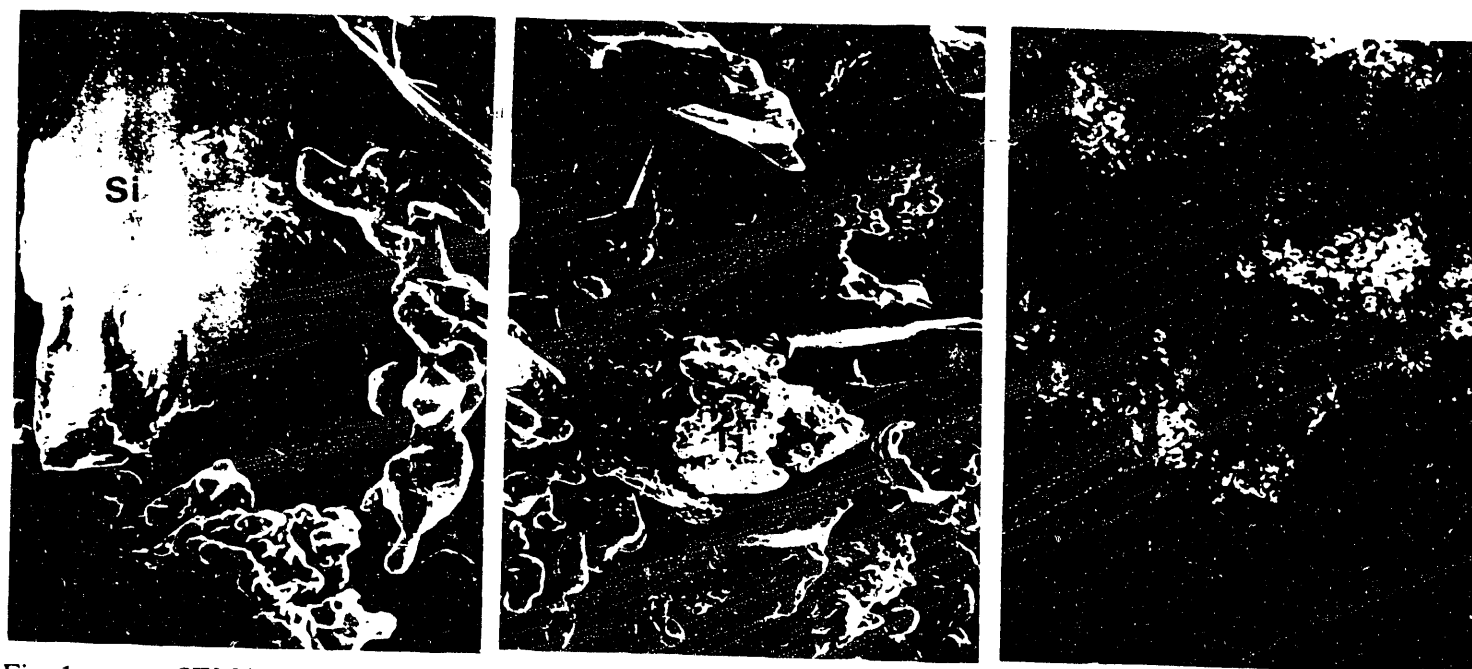


Fig. 1. SEM images showing morphologies of Ti-Si powder mixtures: (a) **coarse** (b) **medium**, and (c) **fine** powders. Si particles are generally blocky single crystals and have a shiny contrast, while Ti particles are rounded polycrystalline aggregates with grainy contrast.

## RESULTS

The overall results of shock recovery experiments, characterized based on optical and SEM analysis are illustrated in the reaction map in Figure 2. For **medium** morphology powders, MB-B experiments showed complete reaction in samples with 47% porosity, and no reaction in samples with 36% porosity. The PB-B experiments showed no reaction in samples with 41% and 47% porosity, but complete reaction with 55% porosity. The reaction trends for **medium** morphology powders were used to guide experiments on **fine** and **coarse** morphology powders. However, no reactions were observed with **coarse** powders for MB-B experiments with 47% porosity, and PB-B experiments with 55% porosity. Likewise no reactions were observed with **fine** powders for PB-B experiment with 55% porosity, while only localized reactions in peripheral edge regions of the compacts were observed for MB-B experiment with 47% porosity.

Time-resolved experiments (discussed elsewhere in this proceedings) were performed primarily on **medium** morphology Ti-Si powders at shock pressures up to 3 GPa. The results of time-resolved experiments concur with the recovery experiments, and provide clear evidence of the occurrence of *shock-induced chemical reactions* in Ti-Si powder mixtures.

In general, the microstructure of the fully reacted samples showed an equiaxed grain structure, along with presence of spherical voids, typical of a fully reacted, melted, and resolidified material. The size of the equiaxed  $\text{Ti}_3\text{Si}_2$  grains was measured to be  $\approx 10 \mu\text{m}$ . A typical fully reacted microstructure is shown in Figure 3.

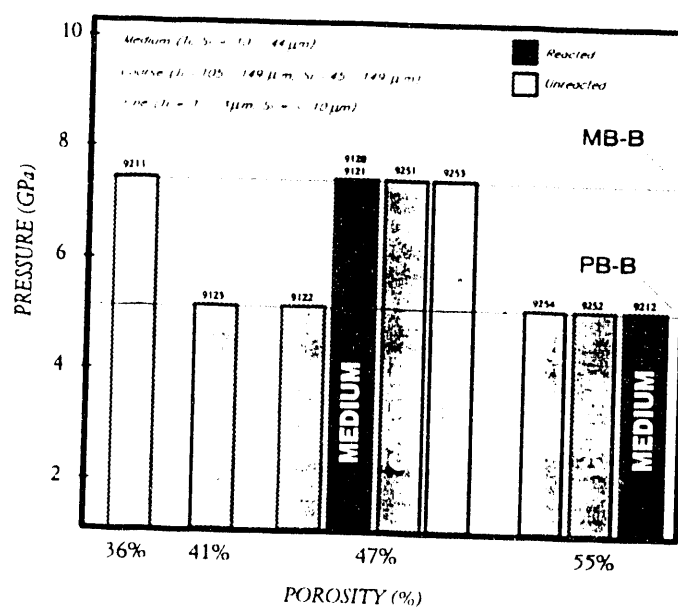


Fig. 2. Reaction map showing effect of initial density, powder morphology, and conditions.

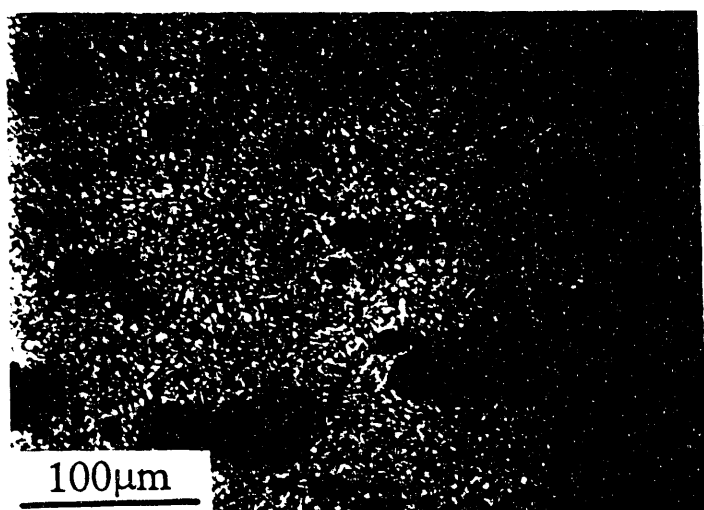


Fig. 3. Optical micrograph showing fully reacted microstructure.

Unreacted samples from experiments performed at shock conditions below the threshold are of principal interest in the present work. Such samples provide the configuration of powder mixtures in the shock-compressed state at various stages prior to inception of reaction. In order to compare the microstructure resulting from the effects of different variables, analysis was performed along identical regions of every microstructural compact, namely the central bulk area.

The most revealing effects are observed in samples of the three different morphologies, packed at similar density in the PB-B shock recovery fixture; the three corresponding optical micrographs are shown in Figure 4 (a-c). The grainy-contrast **fine**, **medium**, and **coarse** morphology Ti particles in all cases show extensive deformation. The **fine** morphology Ti particles are also seen to form large agglomerates  $\approx 200 \mu\text{m}$  diameter. The shiny-contrast **fine** morphology Si particles show extensive deformation and flow around Ti particles (Fig. 4(a)). On the other hand the shiny-contrast **coarse** Si particles show extensive fracture and fragmentation (Fig. 4(b)). The **medium** morphology Si powders show some cracking, as well as deformation and flow, the latter case observed particularly when Si is isolated and surrounded by Ti particles (Fig. 4 (c)).

The effect of shock pressure was best revealed on **medium** morphology Ti-Si powders. Optical micrographs of powders shock-compressed with the low pressure PB-B fixture and the higher pressure MB-B fixture are shown in Figure 5 (a,b). While extensive deformation of the grainy-contrast Ti particles is commonly observed in both micrographs, the mixtures shock-compressed with the higher pressure MB-B fixture (Fig. 6(b)) show more cracking than the those with the PB-B fixture. There is also evidence of possible melting of Si, in certain localized regions of the MB-B samples.

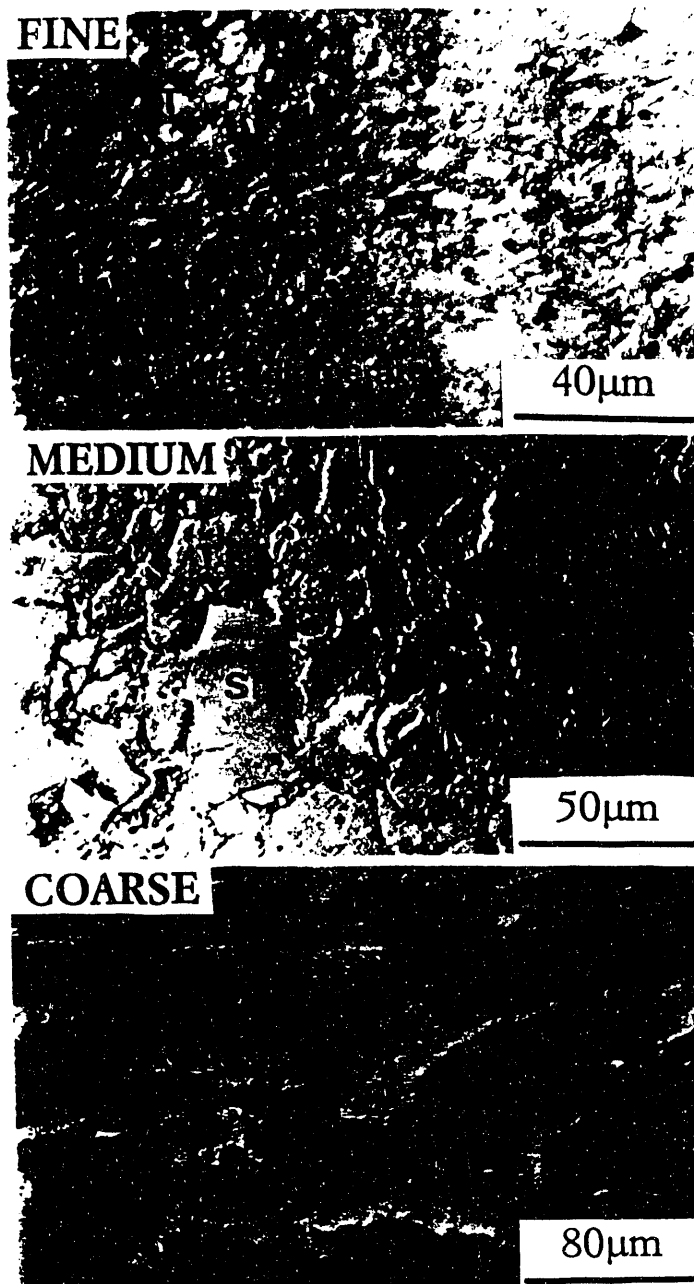


Fig. 4. Optical micrographs of **fine**, **medium**, and **coarse** morphology powders shock compressed with PB-B fixture at same packing density.

## DISCUSSION

The overall scenario revealed by recovery experiments illustrates that *shock-induced chemical reactions* in Ti-Si powder mixtures occur predominately with **medium** morphology powders. The reaction thresholds for **medium** morphology powders are shock conditions generated with PB-B system with initial porosity of 55%, or with MB-B system and 47% initial

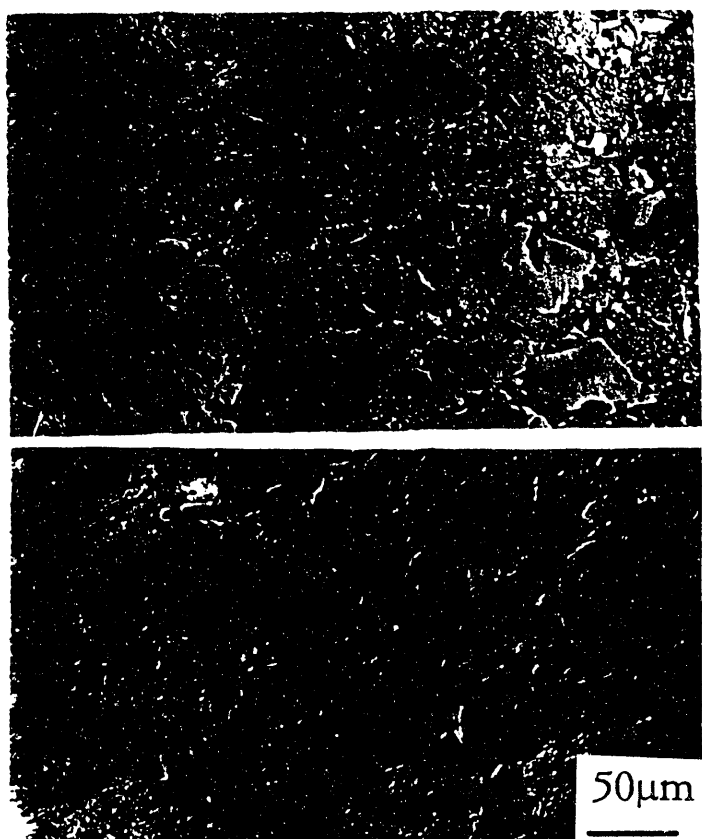


Fig. 5. Optical micrographs of powders shock-compressed with the low pressure PB-B fixture and the higher pressure MB-B fixture.

porosity. The picture emerging from the shock-compressed unreacted configuration of Ti-Si powder mixtures provides clues of mechanistic processes that cause reactions in **medium** morphology powders and not in **fine** or **coarse** morphology powders. As shown in the micrographs in Figures 4 and 5, both Ti and Si **medium** morphology powders simultaneously undergo extensive deformation and flow leading to more intimate mixing between them. In contrast **coarse** morphology Si powders fracture and fragment at low stresses, prior to deformation of Ti particles, therefore, there is only limited mixing between the deformed Ti and Si fragments. **Fine** morphology Ti and Si powders are expected to undergo extensive deformation, and therefore the greatest propensity for reaction initiation. However, while **fine** Si particles do show extensive deformation and flow, the **fine** Ti particles tend to agglomerate, thereby limiting interparticle mixing.

#### *Mechanistic Considerations*

*Simultaneous deformation of constituents* is therefore, the important property needed to provide an ideal configuration for initiation of *shock-induced chemical reactions*. Morphological variations and

porosity affect reaction initiation characteristics, by altering simultaneous deformability of the constituents. The deformation response of Si is also different when it is shock-compressed with other metals in a binary mixture, e.g., with Ni, Nb, Mo, instead of Ti. Prior work<sup>5,6</sup> shows that Ni-Si and Ti-Si systems have the highest propensity for reaction initiation, while Nb-Si and Mo-Si systems have the lowest propensity. The Ni-Si and Ti-Si systems are favored because of the small difference in the yield strength of constituents which allows simultaneous deformation, plastic flow, and mixing to occur. In contrast, large yield strength differences amongst constituents in Mo-Si and Nb-Si, inhibit complete mixing since the metal constituent has to deform at higher stresses, and then mix with fragments of the brittle Si. Thus, simultaneous deformation and mixing is the first step towards providing the configuration for initiation of *shock-induced chemical reactions* consistent with Graham's CONMAH model<sup>7</sup>.

#### SUMMARY

Shock-induced chemical reactions in Ti-Si powder mixtures occur at lower thresholds with **medium** morphology powders. In contrast, mixing is inhibited with **coarse** and **fine** powders due to fragmentation or agglomeration problems which limit the propensity for reaction initiation. Effects of powder morphology, initial porosity, and shock conditions, on resulting microstructure of shock-compressed unreacted Ti-Si powders, reveal the importance of the deformation response of Si, and its subsequent mixing with Ti, in providing the configuration needed for reaction initiation.

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