A New Dynamic Powder Consolidation Technique Using Shock Waves

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Techniques for shock consolidation of powders have been developed for different purposes, including the synthesis of diamond from carbon powder. In this work, a new device configuration for dynamic consolidation is proposed. It consists of three coaxial tubes, with a conical cover made of explosive at the top of the device. The inner tube contains the powder to be compacted. The second is accelerated towards the first in order to promote its collapse. The third confines the explosive. A conical cap at the top of the device triggers the explosive. For a preliminary evaluation, two types of explosives, TNT and Composition B, were used. Preliminary analytical results by the impedance matching method indicate that maximum pressures of 35.44 GPa and 48.16 GPa could be achieved using TNT and Composition B, respectively. Maximum temperatures around 1,600 K and 2,500 K for TNT and Composition B, respectively, are expected. These pressure and temperature values are adequate for transforming graphite into diamond. Preliminary Rietveld refinement indicated that nanodiamond is a fraction of approximately 54% of the detonation resulting powder.

Keywords: consolidation, detonation, synthesis, dynamic compression.

1. Introduction

Shock wave consolidation and synthesis of materials has been investigated since 1960’s1-14 for many purposes, including the synthesis of diamonds from carbon powder15-27. This process is associated with the use of explosives. Upon detonation, a high-pressure shock wave is generated that moves into the main explosive, initiating the reaction. Figure 1 presents a detonation wave scheme. The front of this wave moves toward the unreacted material with a speed D. The interface between the unreacted explosive and the front of the detonation wave has a high peak pressure, called the von Neumann peak, which is narrow and quickly attenuated. Between the unreacted explosive and detonation of the explosive products, there is a region named chemical reaction zone. It performs the transformation of solid explosive into gaseous detonation products.

The interface between the chemical reaction region and the detonation products is where the synthesis is completed. This is called the Chapman-Jouguet point (C-J), used to characterize the explosive, i.e., its pressure (P C-J) and particle velocity (U p C-J). The wave of relaxation, known as Taylor wave, propagates into the product immediately behind the detonation wave28. The phenomenon of dynamic deformation at high rates due to detonation shock wave is governed by conservation relationships that were derived from Rankine-Hugoniot28-31. The following equations represent, respectively, the conservations of mass, momentum and energy.

\[
\rho_0.D = \rho.(D - U_p). \quad (1)
\]
\[
(P - P_0) = \rho_0.D.U_p. \quad (2)
\]
\[
(E - E_0) = U_p^2/2 + Q. \quad (3)
\]

where \(\rho_0\) is the initial specific mass; \(\rho\) the final specific mass; \(D\) the detonation wave velocity; \(U_p\) the particle velocity; \(P\) the final pressure; \(P_0\) the initial pressure; \(E\) the final energy; \(E_0\) the initial energy; \(V\) the final volume; \(V_0\) the initial volume, and \(Q\) is the chemical energy per mass unit.

The conservation equations, (1), (2) e (3), involve 5 variables. So, one additional equation is required to relate them. Then, it is also used an experimentally obtained equation of state shown in Eq. 4.

\[
U_p = C_0 + S.U_p. \quad (4)
\]

where \(S\) is an empirical parameter and \(C_0\) a characteristic sound wave velocity.

Some previous methods use substantial amounts of explosives, in the order of up to hundreds of pounds. Besides that, there are methods that combine distinct types of explosives which can generate difficulties, such as good interaction of different explosives, and interface effects as well. With the present method, only about 2 kg of a single type of explosive was used in each detonation for similar
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purpose. This contributes to minimizing the cost of confection of the device, including the amount of explosive, making it possible to increase the number of tests to be performed.

2. Materials and Methods

As aforementioned, this new configuration is proposed to transform a carbon precursor powder into diamond. Then, as such precursor, carbon black (Quimesp, 98% purity) was used. Upon transformation, a fast quench is necessary to maintain the diamond structure. Thus, copper powder (Viner Brasil Tecnologia, 99.6% purity) was chosen as quenching medium, given its known high thermal conductivity. The carbon black and copper powder were mixed, with a weight ratio of 10/90, respectively, to ensure greater homogeneity and satisfactory cooling to achieve the desired transformation.

The new design for dynamic consolidation is a round configuration consisting of three concentric cylinders in the form of tubes. Meyers and Wang were the first to use this technique with the purpose of promote powder synthesis by shock wave. Subsequently, Ferreira improved it. From the device successfully used by Meyers, an adaptation has been made, shown schematically in Figure 2. This new design requires less explosive and successfully yields comparatively more diamonds than previous ones. This novel technique here proposed is the startup through a single explosive in conical shape at the top of the double tube device. The intermediate cylinder, called flyer tube (diameter of 1.5 in.), is made of the same inner stainless steel tube (diameter of 3/4 in.). The flyer tube is accelerated inward by the shock wave produced by the detonation of TNT (trinitrotoluene) and Composition B (hexolite, 60wt% RDX and 40wt% TNT) that collapse the inner tube containing the powder to be synthesized. These tubes are 304 stainless steel and 300 mm high. High pressure and elevated temperature achieved by the shock wave are favorable conditions for carbon transformation into the diamond structure. Between the steel tubes, there is an empty space that is required for accelerating the flyer tube against the inner tube containing the powder. The external tube, made of PVC, with 500 mm of height and 100 mm of diameter, confines the explosive. The explosives were cast and poured into the device. Then, its solidification was made with the device immersed in flowing water at room temperature.

It is expected that the detonation wave of the conical explosive cap (also with 100 mm diameter), initiated by the detonator, reaches the cap/explosive interface as a plane wave, given the distance to be traveled and the speed of the detonation wave.

The calculation of the pressure generated by the shock wave at the moment of the impact was estimated using the shock impedance matching method. This is given by the intersection of the direct Hugoniot from the target material with the inverted Hugoniot from the impacting material. The relation between the impact velocity of the flyer tube and the ratio of the masses of the flyer tube and of the charge (M/C) follows the Gurney’s equation for cylindrical configuration, presented by Eq. 5.

\[
V_p = \sqrt{2E_p \left[ \frac{5M}{C} + 2\left(\frac{M}{C}\right)\left(\frac{R+\eta}{\eta} + \frac{2\eta}{R+\eta}\right) \right]}.
\]

Figure 1. (a) The structure of a detonation shock wave, and (b) the pressure as a function of time (adapted from Meyers).

Figure 2. Schematic representation of the proposed device (adapted from Meyers), with the conical cap made of explosive.

A sequence of dynamic relationships permitted the evaluation of the pressure at the C-J point.

The \( P \times U_p \) direct Hugoniot of the materials may be calculated by Eq. 6.

\[
P = \rho_u (C_0 + S.U_p)U_p.
\]
and its P x Up inverted Hugoniot, presented as follow.

\[ P = \rho_0 \left[ C_0 + S(V - U_p) \right] (V - U_p). \]  

(7)

were V is the impact velocity. The P x Up inverted Hugoniot of the explosive is given by.

\[ P = \frac{1}{2} \rho_0 (V - U_p) (\gamma + 1) + Q \rho_0 (\gamma - 1). \]  

(8)

and the pressure at the Chapman-Jouguet point \( (P_{CJ}) \) can be calculated by.

\[ P_{CJ} = \rho_0 D^2 / (\gamma + 1). \]  

(9)

where \( \gamma \) is the polytropic gas constant.

3. Results and Discussion

The first results were achieved considering the TNT explosive. All parameters involved were taken from Meyers\textsuperscript{28}. In order to obtain the pressure values in the flying tube \( P_{FT} \) and its respective particle velocity \( (U_p)_{FT} \) as well as the pressure in the copper powder, the values of the intersections of the Hugoniot curves of the materials involved were used, as seen in Figure 3.

Observing the graph, the point that intercepts the direct Hugoniot of the flyer tube with the inverted Hugoniot of the explosive provides \( P_{FT} \approx 36.50 \) GPa and \( (U_p)_{FT} \approx 801.47 \) m/s. One can also observe that the impact velocity of the flyer tube is about 1,602.94 m/s, which, in accord with the Gurney equation\textsuperscript{31}. The dimensions of the device, provides an M/C ratio around 0.885.

The direct Hugoniot of the container of the powder to be compacted (copper with carbon) is hidden by the direct Hugoniot of the flyer tube because both are made of the same material. It is also seen in Figure 3 that the pressure on the mixture powder, due the interaction with the stainless steel tube, was about 36.62 GPa, with particle velocity of 799.23 m/s.

Figure 4 illustrates the direct and inverted Hugoniots of the materials involved in the detonation of the Composition B explosive.

The intersection point of the direct Hugoniot of the flyer tube with the Composition B inverted Hugoniot gives \( P_{FT} \approx 47.85 \) GPa and \( (U_p)_{FT} \approx 999.52 \) m/s. The impact velocity of the flyer tube is about 1,999.04 m/s, providing an M/C ratio about 0.718. Besides that, one can observe that the pressure generated on the mixture of copper and carbon black was about 48.16 GPa, with particle velocity close to 994.46 m/s.

In order to estimate the temperature reached by the detonation, the method described by Meyers\textsuperscript{28} to the temperature rise associated with shock waves was adopted. The standard solution is of the form shown in Eq. 10.

\[
T = T_0 \exp \left[ \left( \frac{V_0}{V} \right) (V_0 - V) \right] + \frac{(V_0 - V)}{2C_v} P + \frac{\exp \left[ \left( \frac{V_0}{V} \right) V \right]}{2C_v} \\
\int_{V_0}^{V} P \exp \left[ \left( \frac{V_0}{V} \right) V \right] \left[ 2 - \left( \frac{V_0}{V} \right) (V_0 - V) \right] dV.
\]  

(10)

According to the values displayed on literature\textsuperscript{28}, a temperature of the order of 1,600 K is estimated for the TNT detonation, and about 2,500 K for the detonation of the Composition B explosive.

Such values of pressure and temperature, even for the TNT and Composition B explosives, achieved the diamond region on the carbon phase diagram presented in Figure 5.
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Rietveld refinement of the products obtained from the TNT explosive detonation was performed. It indicated that a considerable amount of detonation diamonds (more then 50%), with crystallite size about 29 nm, and GOF of 1.418, was achieved as can be seen in Figure 6. Moreover, experimental evidence of transformed diamond nanoparticles is shown in Figure 7.

Preliminary Raman spectroscopy analyses of the detonation product confirmed the presence of diamonds.

4. Conclusions

A different configuration for dynamic compaction of powder is suggested. It consists of a common double tube configuration, with a conical single explosive cap initiation. The pressure, impact velocity and temperature values to be reached with the detonation of explosives were estimated. The shock wave generated by detonation TNT (trinitrotoluene) indicated a pressure around 35.44 GPa and a temperature of approximately 1,600 K, while the Composition B detonation provided a pressure of 48.16 GPa and a temperature of about 2,500 K. By the M/C ratio, it can be seen that the necessary quantity of explosives is relatively small (~2 kg), reducing the cost of the process. The preliminary experimental results of SEM, Rietveld refinement and Raman spectroscopy, confirmed the presence of transformed nanodiamonds, with estimated crystallite size of about 29 nm.

5. References


