Catalytic Detonation of RDX/TNT Blend Explosives for the Assembly of Carbon Nanostructures

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Abstract

Nano-structured materials have been synthesized by a self-heating detonation process using a RDX/TNT blend explosive (i.e. B explosive) for providing the need of high temperatures, high shock waves, and parts of carbon sources in the presence of metallic-containing catalysts. The products of carbon nanomaterials are characterized by SEM, EDX and TEM techniques. The systematic experiments carried out indicate that mixture of RDX/metalcene with or without carbon source as a molecular precursor can be employed to produce transition metals (Fe, Co and Ni) nanoparticles encapsulated in concentric layers of graphitic carbon. Moreover, various pure carbon or metal nanostructures can be simply obtained from the detonation of the desired molecular precursors. Therefore, catalytic detonation of carbon-rich explosives can be designed as a useful method and with the potential application for the production of nano-structured materials of graphitic carbon-encapsulated nanoparticles and carbon-nanotubes. The experimental results show that the metal compounds can be converted into metallic nanoparticles due to the fast decomposition with a reduction reaction after the detonation and this will play an important role for the growth of different size of carbon capsules. The systematic of experiments indicate that it is possible for a cheaper process and can be as an alternative compared to these high energy and hardware intensive processes to assemble nano-sized carbon nanomaterials under catalyzed-blast process.

Keywords: Detonation, Nanostructures, Explosives

1. Introduction

Due to their unique properties, carbon nanotubes (CNTs) are an extremely attractive raw material for functional as well as structural applications. In recent years, dramatic advances have been accomplished, especially concerning the use of CNTs in nano-electronics. For this field of application comparatively small amounts of highly determined CNTs are sufficient to serve valuable functions, which makes relatively high prices tolerable. However, as traditional CNT synthesis like arc-discharge, CVD or laser ablation is energy- and setup-intensive, routes to cheap mass production of CNTs are highly demanded [1-3], especially for their utilization in structural materials, where large amounts are required. The novel structure of encapsulating second phase inside carbon shells can immunize the encapsulated species against environmental degradation effects while retaining their intrinsic properties, and can also offer an opportunity to investigate dimensionally confined system. The synthesis of carbon-encapsulated metal nanoparticles has attracted much attention for their wide promising applications, especially in information technologies and biomedicines. There are many differences among these methods in technique as well as in chemical and physical principles, the common base is that nanostructures always grow under high temperature conditions. However, these processes are both high energy and hardware intensive, which lead to high cost of nanostructures and therefore constrains their practical application [4-6].

Explosive decomposition-experiments and shock wave synthesis of nanoscale materials have been described in literature. These include e.g. the preparation of binary
nitrides such as c-BN, CNx-materials and GaN. Even the commercial fabrication of diamond nanopowders is performed by shock wave methods [8-11]. In this way, uniform iron nanoparticles well encapsulated within graphitic shells can be obtained, with crystalline structure of parent ones. Therefore, a laboratory self-heating detonation process has been designed in-house and a more effective synthesis of CNTs using nitro-amine CHNO explosives as an energetic materials and the metal containing material as a catalyst. Here we report that individual carbon nanostructures, both unfilled and containing metal nanocrystals in a string-by-string bead-like arrangement, can be obtained reproducibly by detonative decomposition of a RDX/TNT explosive.

2. Experimental

The chemical reagents used were RDX/TNT energetic materials (B explosive), transition metal catalysts (Co, Ni, and Fe containing compounds) and anthracene (C_{14}H_{10}). The use of this specially system to study the catalysis-assisted detonation process, the relationship between the experimental conditions and product distribution and roles of the catalyst types. Before the detonation experiments, the starting materials were mixed in desired ratios. The detonation was performed in a sealed stainless steel vessel connected with vacuum and inert gas control system, and induced external heating to ignition temperature. After the detonation, the reactor was cooled in air to room temperature. The gaseous products were vented and the solid products were collected for further characterizations. The reactor and various units of the collection system were weighted before and after the runs to determine the mass balance. Scanning Electron Microscopy with detection ) SEM equipped with EDX and Transmission electron microscopy (TEM) were employed to investigate the as-synthesized solid products.

3. Results and discussion

An individual metal catalyst was mixed with explosives (RDX) before the detonation experiments. The materials used in this study can be formulated, including explosive, carbon source, and catalyst, from which carbon nanomaterials can be effectively synthesized. Fig. 1 is a typical XRD result of the sample obtained from the detonations of RDX-Fe mixture. XRD characterization is performed to further validate the corresponding structure of the core and shell. No signals of iron carbide or iron oxide are observed. Although it is difficult to completely rule out the presence of very small oxide and carbide particles from the XRD pattern because the particles possessing a scattering region smaller than 2 nm cannot be registered with the X-ray technique. TEM observation shows that the size of the particles are larger than 5 nm, suggesting the cores will be bcc-Fe. The diffraction peak at about 26.2° can be assigned to the (002) planes of hexagonal graphite structure with an interlayer spacing of 0.34 nm, corresponding to the encapsulating carbon shells. The peak is rather asymmetry, broader and lower than that of the well-crystallized graphite, indicating a relatively small crystalline dimension. Amorphous carbon background in the products contributes to the broad diffraction peak in proximate to the graphite peak. A typical TEM image of the resulted material showing that the Fe–C core–shell structures with the carbon shells show relatively defective structure observed can be effectively protect the iron cores against the environmental degradation (Fig. 2). The iron cores are crystal and have lattice fringe spacing of 0.20 nm), related to the (110) plane of the bcc-Fe crystal or the (121) plane of the Fe_{7}C_{3} crystal. The identification of the phase can be realized in virtue of XRD measurements (Fig. 1).

As shown in Fig. 3, it indicate that the mixture result in catalytic detonation reaction and produce nanostructures under the condition. The above data show that the detonation-induced Co pyrolysis is able to controllably produce well-constructed Co–C core–shell nanostructures. In this process, since the detonation of RDX is induced by temperature-programmed heating. The hot gases (N_{2}, CO, CO_{2}, H_{2}O) generated from the detonation collide with the gaseous molecules and make latter quickly decompose into small carbon (Cn) and Co species, which subsequently condense into solid materials when cooling. The simultaneous condensation of the Co clusters and the Cn species leads to the likely formation of a (Co, C) alloy, whose carbon content varies with the system temperature. When the carbon dissolution in the Co nanoparticles reaches saturation, a precipitation of pure carbon around the nanoparticles would start in the form of graphite.
Fig. 4 shows typical TEM patterns of the as-synthesized samples obtained from the detonations of RDX/Nickelocene/C_{14}H_{10} mixture. The presence of Ni catalyst is necessary for the nanostructures growth in this system, at least under the experimental used in this study. TEM image of this sample presents the effect of C_{14}H_{10} addition on the formation of carbon nanotubes. Elemental analyses by EDX show that the products mainly consist of carbon and catalyst with very little amount of detectable oxygen and nitrogen. Both of the recipe RDX/Nickelocene/C_{14}H_{10} and RDX/cobaltocene/C_{14}H_{10} of the TEM micrograph in Figs. 4 and especially in Fig. 5 show that the length of the tubes can reach more than a dozen microns and that they are segmented. The term “bamboo-like nanotubes” has been introduced for this nanostructures morphology. Based on theoretical studies it was supposed that nitrogen substitution of carbon in graphite develops buckled structures and enhances the compartmentization of nanostructures. However, a detailed and possibly quantitative experimental investigation of the influence of nitrogen incorporation on the morphology of carbon nanostructures remains to be conducted in the future. The segment of long tube in Fig. 5 has diameters of about 50 to 100 nm (right). Similar to the left figure shown that all produced materials the tube diameters vary between 100 and 150 nm. All tubes prepared with Co transition metal and carbon sources (C_{14}H_{10}) were multi-walled with the said dimensions. The morphology and the nanostructures yield varied depending on the metal. As can be seen in Fig. 6, in the formation of the nanostructures of nanoparticles of nanoencapsule (right) and nano-sized metal particles (Left), the explosive detonative plays an important role with the heat and the carbon species produced from the detonation promote the decomposition and the reduction of catalyst particle and this lead to help the structure and mechanism control. The core area in HR-TEM image reveals the lattice fringe spacing of the core is about 0.20 nm with Fe–C core–shell structure can be formed selectively in the present approach via simply controlling the ratio of RDX/Ferrocene. The shells are uniform in thickness and usually consist of 5–18 layers. The spacing of the lattice fringes is about 0.34 nm, which is close to that of the graphite (002) planes. It is interesting to note that these results experimentally used in this study show that it is possible for a cheaper process and can be as an alternatives compared to these high energy and hardware intensive processes to assemble nano-sized carbon nanomaterials under catalyzed-blast process.

4. Conclusion

The detonation of nitro amine-containing CHNO explosive as common as a RDX/TNT composite can be used to synthesized carbon nanomaterials in the presence of a catalyst. The approach has the potential ability to convert waste energetic explosives to form highly valuable materials. This method represents a novel and low cost process towards metal–carbon encapsulating structures, in which the needed high-temperature environment is self provided by the energy emitted from the RDX/TNT detonation. sing this special system prticulate products are generated. Similar results were obtained when the reaction was performed in a certain outward flow of gaseous reaction products and intermediate pressure decline rates, and in the presence of iron, nickel or cobalt, various nanostructures are formed. Uniform carbon-encapsulated Fe nanoparticles are successfully synthesized through the detonation of RDX/TNT and metalocene mixture. For the controlling formation of carbon-encapsulated metal nanoparticles and carbon nanotubes, it is clear that C:metal ratio in the starting materials is considerable controled to obtain the majority of high yields of encapsulated metal nanoparticles without the formation of carbon nanostructures. A further increase in caobon nanostructures yield and tailoring of structure defects may be available in relation to the optimization of reaction conditions.

References


Fig. 1. XRD spectrum of catalytic detonation of RDX over Ni, Co and Fe catalysts.

Fig. 2. TEM image of the catalytic detonation of RDX/TNT over a Fe catalyst (1:1).

Fig. 3. TEM images of the catalytic detonation of RDX/TNT over a Co catalyst (1:1).

Fig. 4. TEM images for the catalyzed-blast of RDX/TNT a Ni catalyst (1:1).

Fig. 5. TEM images for the catalyzed-blast of RDX/TNT /Cobalcene/C14H10 mixture.

Fig. 6. HRTEM images of for the catalytic detonation of RDX/TNT explosive with Ni catalyst (10:1).