



Effect of surface coatings on aluminum fuel particles toward nanocomposite combustion

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ABSTRACT

Flame front velocity (FFV) of three energetic material composites was measured in order to understand the effects of surface functionalization on aluminum reactivity. Composites were prepared using molybdenum trioxide (MoO₃) and aluminum (Al) fuel particles with and without surface functionalization. The surface functionalization consisted of a 5-nm-thick layer (35% by weight) of perfluorotetradecanoic acid (PFTD) bonded to the Al₂O₃ surface of the Al particles. The first composite consisted of Al functionalized with PFTD and MoO₃, the second consisted of Al with MoO₃ and added PFTD particles to the same weight percentage as in the Al functionalized PFTD, and the third composite consisted of Al with MoO₃. The results showed a dramatic increase in FFV from 100 to 500 m/s resulting from the surface functionalization. The results of the experiments show that the surface functionalized Al composite (Al-PFTD/MoO₃) has a reaction rate 2× than that of the simple Al/MoO₃ and 3.5× than that of the Al/MoO₃/PFTD composite.

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1. Introduction

Energetic materials can be classified as monomolecular or composite. Monomolecular energetic materials contain fuel and oxidizer atoms bonded within a molecular structure. Their reaction is limited by the kinetics controlled by bond energies. Composites generally are a mixture of discrete reactants. Pyrotechnics and thermites are examples of composites that combine a fuel with an oxidizer to form an energetic composite. The oxidation process for thermites is diffusion limited such that the mass transport and diffusion distances control the energy release rate. A reduced reactant size, from micron to nanoscale, translates to lower diffusion distances, increased surface area to volume ratio for individual particles, increased number of contact points between the fuel and oxidizers, and hence increased reactivity and reaction rate [1–4].

There are however several problems associated with the use of nanoscale reactants, e.g., excessive particle agglomeration [5], increased viscosity in solvents [6], and increased sensitivity. In addition, nano-Al particles, which are a preferred fuel for composite formulations because of their high heat of combustion, have a passivating alumina (Al₂O₃) shell with an average thickness of 1.7 to 6.0 nm [7], which can account for as much as 40% of the mass, depending on the particle size. This may be a hindrance to the reactivity of the composite since most oxidizers react only with the Al core and not the passivating alumina shell.

Prolonged exposure to air or moisture will further oxidize the Al particle, thus depleting the active Al content over time, thereby decreasing the energy content and reactivity of the fuel [8].

Several efforts have been made to protect the active Al core in an organic corona to mitigate the effects of the alumina shell [6]. Such an approach was demonstrated by the surface functionalization of the alumina shell by the application of an organic coating over the Al core without Al₂O₃ shell [6].

Composites can be prepared by physically combining the reactants for a given stoichiometry using solvent based ultrasound, sol-gel, or dry mixing techniques to achieve an intimate mixture of fuel and oxidizer. In any case, the purpose of the mixing process is to physically homogenize the composite, decrease the density and chemistry gradients in the mixture, and increase the points of contact between the fuel and the oxidizer components. A recent approach has been to synthesize composites using a self-assembly process [9–12]. Self-assembly results in orderly arrangement of the fuel and oxidizer species typically in solvent. Research has shown that the thermal behavior and general performance of self-assembled composites has consistently surpassed those prepared by physical mixing [9–12].

Surface functionalization of oxidizer moieties on a fuel particle is one example of self-assembly. In the case of aluminum, the particle has an Al₂O₃ shell, so the material used for surface functionalization should be capable of interacting either physically or chemically with the shell. Under standard atmospheric conditions, the Al₂O₃ shell can become partially hydroxylated [13], providing an additional route for surface functionalization. Ample literature is available about the chemical functionalization of Al₂O₃ on bulk Al particles using the condensation

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Table 1
Physical and chemical specifications of the reactant materials.

| Material | Manufacturer | Average particle size (nm) | Oxide layer thickness (nm) | Acid layer thickness (nm) | Particle morphology |
|------------------------|-----------------------|----------------------------|----------------------------|---------------------------|-------------------------------|
| Al | Novacentrix | 80 | 2.7 | N/A | Spherical |
| Functionalized Al-PFTD | NSWC, Indian Head, MD | 80 | 2.7 | 5 | Spherical with SAMs |
| PFTD particles | SynQuest Technologies | <44 μm | N/A | N/A | Polymer chains |
| MoO ₃ | Mach I | 44 | N/A | N/A | Rectangular plate-like flakes |

of carboxylic acids to surface bound hydroxyls in order to form self-assembled monolayers (SAMs) [14–16]. Surface functionalization of alumina with silanes [13], phosphoric acids [14], and hydroxamic acids [17] has been demonstrated for diverse applications. Research shows that the physical properties of these nanoparticles can be influenced to a great extent through modification of the chemical composition of the surface corona [12,18,19]. The current work employs the use of aluminum particles functionalized with self-assembled monolayers of organic acids for a unique application involving energetic materials.

Previous work showed that the addition of perfluoroalkyl coronas to Al fuel particles affected the FFV and apparent activation energy of the Al particle depending on the acid chosen to functionalize the fuel particles [12]. In contrast to physically mixed composites, surface functionalized Al particles have oxidizers chemically bonded to the fuel [21]. In this way, composites containing functionalized Al fuel particles should exhibit reaction behaviors that can be similar to or associated with monomolecular energetic materials. Comparing the reaction rate of composites prepared from the chemically modified Al to composites prepared with unmodified Al is the objective of this study.

2. Experimental

Identical Al particles with 80 nm average particle diameter were used as fuels in this study. All the Al particles were encapsulated in an alumina (Al₂O₃) passivation shell with an average thickness of 2.7 nm. Surface functionalization of the Al results in a 5-nm-thick layer (35% by weight) of perfluorotetradecanoic acid (PFTD) bonded to the Al-Al₂O₃ core-shell particle. The detailed preparation method for the acid-coated Al particles may be obtained elsewhere [21]. The second type of Al particles had an alumina passivation shell without acid coating and will be referred to as Al. Molybdenum trioxide (MoO₃) is used as the principal oxidizer. Table 1 consists of material details used in this study.

The three different composites, identified as Al/MoO₃/PFTD, Al-PFTD/MoO₃, and Al/MoO₃, prepared for the flame propagation experiments, are identified in Table 2. Al/MoO₃/PFTD is a physical mixture of Al, PFTD powder and MoO₃. Al-PFTD/MoO₃ is composed of MoO₃ and Al particles coated with PFTD acid chains. Al/MoO₃ consists of Al and MoO₃ alone. The redox reactions between Al, the acid shell, and MoO₃ are complex; hence, the reactant concentrations are expressed in terms of mass percentages and not in terms of equivalence ratio. Birce et al. [20] showed that similar Al-PFTD/MoO₃ combinations with 70.6% by mass MoO₃ have the highest FFV and the same Al-PFTD/MoO₃ ratio was adopted here. Since the Al-PFTD particles had 35% by mass of PFTD, the PFTD content accounted for 10.36% of the total Al-PFTD/MoO₃. This implied that the active Al and the Al₂O₃ content in Al-PFTD accounted for 19.06% of the total composite mass. The same mass percentages were assumed for preparing the Al/MoO₃/PFTD composite

too in order to keep the chemistry of the reaction constant and vary only the proximity of the PFTD acid to the Al in order to study its effects on the burn velocity of the composites. The mass percentages of fuel and oxidizers present in the three different composites prepared are given in Table 2.

Measured quantities of reactants required for preparing each composite were suspended in hexanes. The suspension was then sonicated using a Misonix Sonic wand for 120 s in 10-s intervals to break agglomerates and improve homogeneity of the composite. The hexanes suspension was transferred to a Pyrex dish and heated to a temperature of 45 °C to facilitate the evaporation of hexane. Once the powder mixture dried, it was reclaimed for further experimentation.

The prepared composites were subjected to flame propagation experiments to determine their FFVs. A schematic of the experimental set up is shown in Fig. 1. It consists of a quartz tube, 110 mm long, with an inner diameter of 3 mm and an outer diameter of 8 mm. Each composite was loaded into the quartz tube and placed on a vibrating block for 5 s to reduce local density gradients. Each tube contained approximately 468 ± 10 mg of composite resulting in a loose powder fill estimated to be 7% of the theoretical maximum density. Once prepared, the tube was placed in a steel combustion chamber with viewing ports for diagnostics. Three quartz tubes were prepared for each composite allowing for an estimate of the repeatability and uncertainty in the measurement.

Ignition was achieved via thermal stimulus provided by a Nichrome wire connected to an external voltage supply. A Phantom v7 (Vision Research, Inc., Wayne, NJ) with a Nikon AF Nikkor 52 mm 1:2.8 lens was used to record ignition and flame propagation. The camera captured images of the reacting composite, perpendicular to the direction of flame propagation, at a speed of 160,000 frames per second, with a resolution of 256 by 128 pixels. Vision Research software was used to post-process the recorded photographic data. When a reference length is established, the software determines speed based on a distance between sequential time frames. Using a “find-edge” image filter that identifies preset variations in pixel intensity, the flame front location (which is identified as the region of the flame with the maximum radiance) is identified and marked for speed measurements.

3. Results and discussion

Fig. 2 shows a representative plot for the distance traversed by the flame front as a function of time. The initial portion of the curve shows unsteadiness as the flame progresses down the quartz tube. Flame speed is measured when propagation attains steady state behavior seen in the latter portion of the tube represented by linearity in the distance versus time plot (Fig. 2). The slope of the linear region represents FFV.

The steady-state FFVs are compared in Fig. 3 with bars representing standard deviations. The FFV of the acid-coated aluminum (Al-PFTD/

Table 2
Fuel and oxidizer reactants, along with their masses in the composites prepared.

| Sample name | Fuel | % Fuel in the composite | Oxidizer 1 | % Oxidizer 1 in the composite | Oxidizer 2 | % Oxidizer 2 in the composite |
|---------------------------|---------|-------------------------|------------------|-------------------------------|------------------|-------------------------------|
| Al/MoO ₃ /PFTD | Al | 19.04 | PFTD powder | 10.36 | MoO ₃ | 70.6 |
| Al-PFTD/MoO ₃ | Al-PFTD | 19.04 | PFTD coating | 10.36 | MoO ₃ | 70.6 |
| Al/MoO ₃ | Al | 21.24 | MoO ₃ | 78.76 | — | — |

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