More Bang for Your Buck: How Changing the Chemical Properties of Aluminum Particles Increases their Power

Dr Michelle Pantoya

JANUARY 2025

doi.org/10.33548/SCIENTIA1227



ENGINEERING & COMPUTER SCIENCE







More Bang for Your Buck: How Changing the Chemical Properties of Aluminum Particles Increases their Power

Aluminum particles are widely used in various energy generating applications, such as fuels. However, due to their high reactivity with atmospheric oxygen, they must be coated in a chemical 'shell' in order to prevent spontaneous combustion. This highly protective shell obstructs oxygen from reaching the aluminum core, limiting aluminum's potential to produce power. Dr Michelle Pantoya from Texas Tech University has led a research team to explore alternative shell compositions. New shell chemistry has exciting implications for aluminum use in rocket fuels and other propellants.

## Activating Aluminum: Right Place, Right Time

Aluminum (or aluminium) particles have high chemical reactivity and are energetically dense, leading to their use in a variety of energy generating applications, such as fuels and fireworks. However, pure aluminum particles are highly reactive and will spontaneously combust when in the presence of oxygen in the air, a property that classifies them as pyrophoric. Therefore, they must be chemically encapsulated (coated) in a protective 'shell' that is not reactive, a process called passivation. Usually, a compound called alumina is used, which has the chemical formula Al<sub>2</sub>O<sub>3</sub>. This shell functions as a barrier between the highly reactive inner aluminum core and the external atmospheric oxygen.

However, when the protected aluminum is used in combustion (burning) reactions, the protective shell slows down the process, and only a fraction of the potential power is generated. For instance, although aluminum has 31 MJ/kg (megajoules per kilogram) of potential energy compared to the 14.5 MJ/kg of the well-known explosive TNT, aluminum combustion only releases around 31 kW (kilowatts) of power compared to the 14,500 kW of TNT. Power limitations have spurred research into alternative shell materials that can increase the rate of energy release of aluminum.

Dr Michelle Pantoya of Texas Tech University led a team of researchers in exploring an alternative chemical composition for the protective shell. Previous research has suggested that using a hydrated version of alumina (i.e., by adding water to alumina) produces a compound called bayerite (Al(OH)<sub>3</sub>), which yields much more impressive results than alumina. This led Dr Pantoya to explore the combustion properties of bayerite-shelled aluminum microparticles ( $\mu$ Al), as the smaller aluminum nanoparticles (nAl) used previously have less active aluminum present (and, therefore, are less energy dense than  $\mu$ Al) and also have lower activation energy (meaning they are more sensitive to ignition and pose safety concerns). By focusing on  $\mu$ Al, Dr Pantoya's team aimed to improve the energy release rate, combustion efficiency, and safety. Her team also explored the utility of  $\mu$ Al in propellant fuel, such as rocket fuel, an application that demands high power production.

# **Hydration is Key**

The researchers sought to identify the conditions (i.e., temperature and time needed) to hydrate the protective alumina shell of  $\mu$ Al particles into a bayerite shell, observe the mechanisms by which this hydration is achieved, and examine the burning behaviour of hydrated aluminum particles in a fuel propellant.

The synthesis method to produce bayerite from the original shell compound of alumina involved a process called hydration, in which water molecules were added to the alumina, resulting in the formation of a new compound, bayerite, Al(OH)<sub>3</sub>. To hydrate the alumina shell, the aluminum powder was mixed with water and heated at 35°C while being stirred. To ensure consistent hydration, the temperature was kept constant for the duration of the process. Samples were collected between 17–27 hours and dried at ambient temperature to study the progression of the shell hydration. They used several methods to explore the structure and properties of the compound, including microscopy, spectroscopy, x-ray diffraction and thermal analysis.

Microscopy was used to observe the spherical shape of the particles and confirm the core-shell structure. Tools like spectroscopy, X-ray diffraction, and thermal analysis allowed investigations into the alumina shell conversion into bayerite and to track the chemical transformations over time. These techniques also helped determine how much of the aluminum core was left intact after the hydration reaction, showing that the core remained mostly unaltered. As the aluminum core is a highly reactive component, keeping an intact core is important for producing a powerful reaction. Burn rate trials were also conducted to analyse



the difference in burn rates between standard  $\mu$ Al with alumina shells, and hydrated  $\mu$ Al with bayerite shells at different pressures, providing valuable insights into their combustion behaviour and inferred efficacy in fuels.

#### Shed the Shell, Keep the Core

Dr Pantoya tested methods of chemically hydrating the alumina shell of aluminum particles using water-based solutions to transform the shell into bayerite. This change helps oxygen reach the aluminum core more easily, making the particles burn faster and more efficiently. Importantly, the team achieved this transformation while keeping 96% of the aluminum core intact, which is crucial for preserving the energy content of the particles.

Burning tests showed that the bayerite-coated particles produced from the hydration reaction burned 17.75% faster than the standard, alumina-shelled particles. This improvement was especially noticeable under high-pressure conditions, where the reaction rate and burn efficiency were significantly higher. Increased burn rates make the bayerite-coated particles ideal for uses like rocket propellants, where fast, efficient burning is critical. The bayerite shell also released oxidising gases close to the aluminum core, which improved combustion by providing oxygen exactly where it was needed. Additionally, the enhanced burn rate was accompanied by a reduction in combustion time, allowing for faster energy release and, therefore, greater power production.

Going further still, other tests showed that the bayerite-coated aluminum particles burned more completely, leaving behind less unreacted aluminum after the combustion reaction took place. Overall, the researchers confirmed that turning the alumina shell into bayerite not only sped up burning but also improved how efficiently the particles reacted. Surface modification of metal particles, like aluminum shown here, is a strategy for harnessing unfathomable power. Coating chemistries provide a canvas of new opportunities to produce power, making metal particles ideal for high-performance applications like propulsion systems.

#### **Advantageous Applications**

Dr Pantoya and her team have demonstrated that, through heating alumina-shelled aluminum in water, a hydrated version, bayerite, is produced. This compound provides a shell for aluminum particles that not only prevents them from spontaneously combusting but can also significantly improve their power generation capability compared to alumina-shelled aluminum, making them more effective for energy and propulsion applications.

By increasing the burn rate of aluminum particles, the surface hydration process makes the particles burn faster, improving their power-generating efficiency in energetic applications such as propellants, explosives, and even fuel cells. The ability to achieve this transformation while maintaining the integrity of the aluminum core (preserving 96% of the original material) ensures that the energy density of the particles is retained, making them a more sustainable and efficient alternative to traditional materials.

In addition, the research provides valuable insights into the role of the shell material in the combustion process. The bayerite shell's ability to release oxidising gases near the aluminum core ensures a more controlled and efficient burn, reducing wasted energy. The exciting results from Dr Pantoya's research pave the way for the development of next-generation propulsion systems with improved performance and environmental sustainability.

# "

By increasing the burn rate of aluminum particles, the surface hydration process makes the particles burn faster, improving their power-generating efficiency in energetic applications such as propellants, explosives, and even fuel cells.





# **MEET THE RESEARCHER**

# Dr Michelle Pantoya Mechanical Engineering Department, Texas Tech University, Lubbock, TX, USA



Dr Michelle Pantoya earned her MS and PhD in Mechanical Engineering from the University of California, Davis. After serving as Combustion Program Manager for the California Energy Commission, she joined Texas Tech University in 2000, where she founded the Energetic Material Combustion Lab. The lab supports 20 researchers and has produced over 30 PhD and 50 MS graduates, with an impressive 90% entering the energetic materials field. Her work focuses on safer, more effective energetic materials through synthesis and combustion analysis. With an impressive publication history, Dr Pantoya has coauthored 200+ publications, holds four patents, and has written multiple technical books and chapters. Dr Pantoya is also an active advocate for early STEM education. She has authored award-winning children's books like Engineering Elephants and developed PBS Kids segments. As a certified Engineering is Elementary (EiE) educator, she leads teacher workshops while helping to integrate engineering into curricula for children between the ages of 5 and 14.

# CONTACT

michelle.pantoya@ttu.edu http://www.depts.ttu.edu/combustionlab/ @TexasTech



Whitacre College of Engineering Department of Mechanical Engineering

# **KEY COLLABORATORS**

- Drs Jennifer Gottfried and Chi-Chin Wu, Army Research Laboratory, Aberdeen Proving Ground, Maryland, USA
- Dr Igor Altman, Naval Air Warfare Center, Weapons Division, China Lake, California, USA
- Dr Adelia Aquino, Texas Tech University, USA
- Dr Daniel Tunega, University of Natural Resources and Life Sciences, Vienna

## FUNDING

US Army Research Office grant number W911NF-22-2-0168 is gratefully acknowledged.

## FURTHER READING

MI Malek, W Benson, JD Pantoya, *et al.*, <u>Synthesis of Bayerite</u> <u>Passivated Aluminum Particles and their Combustion in</u> <u>Solid Propellants</u>, *ACS Applied Engineering Materials*, 2024, 2, 1603-1611. DOI: <u>https://doi.org/10.1021/acsaenm.4c00161</u>

JL Micus, C-C Wu, SD Walck, et al., <u>Hydration-Induced Plasma</u> Surface Modification of Aluminum Nanoparticles for Power Generation in Oxygen Deficient Environments, Surface & Coatings Technology, 2024, 488, 131054. DOI: <u>https://doi.org/10.1016/j.surfcoat.2024.13105</u>4

IM Malek, C-C Wu, SD Walck, *et al.*, <u>Hydration of alumina</u> (Al2O3) toward advancing aluminum particles for <u>energy generation applications</u>, *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2022, 652, 129740, DOI: https://doi.org/10.1016/j.colsurfa.2022.129740

Find out more at **scientia.global**