Nanoenergetic Material (nEM) Performance, Aging, and Sensitivity

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What energetic materials are needed?

- Improved “performance”
  - Energy?
    - Composites offer 2-3x
    - Reactive structures could add energy to target
    - Is nanoscale needed for all cases?
  - Power?
    - nEM higher power than classic composites but detonating HE has extremely high power
    - Tunability/switchability is an attractive possibility
  - Other metrics?
    - Combustion characteristics ($r_b$, ignition, quenching), detonation properties, specific impulse, environmental issues (green), DAY, ...
How can improved performance be obtained?

- Can materials be tailored for desired performance?
  - Some control possible with configuration of materials

- Can modeling be used to better guide development of materials?
  - There is a gulf between molecular-level modeling and macroscale-level modeling
  - Currently inadequate to give significant guidance

- What small-scale experiments best to predict application performance?
  - Full-scale testing often very expensive
  - Is a combined small-scale experiments with modeling the best approach?
Other important factors

- There are show-stoppers
  - Aging
    - Performance must not change with time
    - This can be mitigated
    - How to do accelerated aging?
  - Sensitivity?
    - Insensitive munitions increasingly important
    - Some nEMs are very sensitive
      - Others are acceptable
      - Often, can sensitivity can be mitigated with binders, configuration, etc.
      - Some applications REQUIRE sensitivity (primers, electric matches, etc.)
    - There are serious safety issues for those making new nEMs, especially in “large” quantities
Example: Propellants

- Several studies replacing micron-Al with nAl
  - Extra surface area causes problems
- Recently we (PSU-Purdue) have looked at NM-nAl and H$_2$O-nAl

![Graph showing burning rate vs. chamber pressure for different Al particles](image-url)
Why silicon fuels?
- The oxide layer is only 1-2 nm naturally
- Ageing (oxidation) likely better than Al
- Generally less sensitive than Al
- Reactives could be intimately incorporated in silicon-based microscale devices
- Tuning and switching possibilities
- Some systems produce higher temperatures

Previous work:
- Silicon powders used in some pyrotechnic formulations
- Nanoporous silicon etched in silicon wafers filled with oxidizer & reacted

The combustion of silicon-based composites has not been adequately studied
Can control silicon surface properties

- Self-assembled monolayers can be applied to the surface of silicon, on either nanoporous substrates or silicon particles
  - Oxide layer can be stripped off with HF leaving hydrogen termination *(no similar process for Al)*
  - Possible to bond fluorocarbons to the hydrogen termination before exposure to air producing reactive composite *devoid of unreactive oxide*

- If a thin oxide is allowed to form, the same procedures could be used to coat glass can be used to bond Teflon to silicon surfaces
Our approach is to study reactions in powders first to characterize the combustion

Combustion tube experiments, pressure cell experiments will be used to systematically characterize combustion of various Si-oxidizer systems for the first time

Sensitivity will be quantified also
Nanoporous silicon structures (also considering n-type and p-type silicon) will be made using standard silicon fabrication techniques.

- Develop improved methods for filling nanoporous Si with oxidizers and systematically testing
  - User facilities available at PSU and Purdue
  - “On chip” experiments to be developed

Figure 6. Schematic diagram illustrating the characteristic pore morphologies and typical dimensions as a function of dopant type and concentration.

Searson and Macaulay (1992)
Porous Silicon

About 15% Silicon

Voids to be filled with oxidizer

Higher % Silicon
Porous Silicon

About 47% Silicon

Voids to be filled with oxidizer
Can reactivity be switched or tuned?

- Is field activated combustion possible?
- Carrillo-Heian et al. (2001) examined “field-activated” SHS
  - Ohmic and mass transport effects (niobium silicide system)
- Silicon’s electrical properties can changed by doping (n-type and p-type)
Thank you

Questions?
Future Directions

- Improved small-scale testing that is integrated with modeling to predict performance of specific applications
- Better tailoring of reactives
- Multipurpose materials (e.g., structural reactives)
- Improved diagnostics
- Intimate mixing of nanoscale fuels needed in propellants and explosives
- Microscale applications
- More modeling
  - Bridging molecular to macroscale needed