New Energetic Materials

Discussion group
Reactive nanomaterials: main challenges

- **How far down** “nano” will we go?
  - How far can we go?
  - When does it make sense to stop?
  - ~5 mkm currently used
  - 400 – 500 nm predicted to work for explosives
  - Reaction rates need to be predicted as a function of size
    - Ignition
    - Combustion
  - Efficiency predictions lacking (function of size)
  - Modification of interface to affect kinetics – reactive shells, SHS
  - Very fine scale is not good for reactive structured materials – too fast a reaction, too much gas for initial reaction
    - Need an intermediate step
    - Large particles igniting
    - Materials with multiple scales of mixing desirable
• **How to describe properties** of nanocomposite reactive materials?
  – Physical characterization
    • Tight size distribution
    • Size distribution, morphology, surface area
    • Application dependent – matters for propellants, not for explosives
    • Safety, sensitivity, ESD; friction, impact
      – Correlation between sensitivity and reactivity?
        » Impact sensitivity may correlate with reaction kinetics but not energy
        » For explosives: the correlation is strong (maybe not ESD)
        » Impact sensitivity
        » For composites/nanocomposites: impact sensitivity may be a valuable research tool
        » Mechanism: shear, hot spots
        » Different rate initiation processes (shock wave/hammer)
  – Processing safety (as opposed to final item safety)
  – Bulk energy assessment
    – Bomb calorimetry (with tricks, product analysis)
    – Chemical methods of getting
    – DSC type
  – TMD/porosity
    – Effect on ignitability
    – Energy content/managing energy release
    – Porosity controls sensitivity
    – Two scales on porosity/TMD – inside and outside the particle
  – Experimental reactivity assessment aerobic vs anaerobic reactions
  – Aging
    – Long term stability: nanomaterial itself and final product (interacting with environment and other components)
– Models
  • **Fundamental descriptions** (reactions, mechanics)
    – Molecular dynamics
    – Value in relative ranking reactivity based on comparison with experiment
    – Or not
  • **Performance** modeling
    – Chemical +mechanical processes combined
    – **Simplified integrated models**
    – Value in modeling – macro scale/mesoscale
    – Open area
• Do reaction mechanisms depend on the **initiation**?  
  – Thermal  
  – Continuous reaction does not change depending on initiation  
  – Nano-materials – initiation may constitute the entire reaction  
  – Thermal versus shock  
  – Spark versus laser  

• **Is nanoscale a deciding factor?**  
  – Will the same compositions mixed on the same scale behave identically?  
    • Is manufacturing approach important?  

• How to **correlate lab** evaluations/tests with **performance metrics**?