Fundamentals and Technology of Multifunctional Materials and Devices
Room Sunrise - Session C4

Energetic Materials and Microstructures for Nanomanufacturing

Moderators: Karsten Woll, Karlsruhe Institute of Technology (KIT), Ibrahim Emre Gunduz, Purdue University, USA

2:10pm **C4-3 High Surface Area Silicon Quantum Dots for Energetic Materials***, **Philip M. Guerieri**, N Piekiel, S Adams, M Ervin, C Morris,* U.S. Army Research Laboratory, USA

"On-chip" porous silicon has now been researched for a number of years as an energetic material to augment traditional electronics performance, or provide thrust or actuation in small-scale applications. On-chip porous silicon is ideal for these applications thanks to its high energy density and MEMS fabrication capabilities. However, when you consider that "on-chip" porous silicon is, by its nature, attached to a piece of silicon wafer, the effective energy density when including the mass of the energetic portion and the mass of the inert substrate base, is much lower than the energy density of the energetic material alone. In an attempt to obtain similar performance as on-chip porous silicon, we have fabricated silicon powders with a <5nm (quantum dots) primary particle size for use as a fuel in energetic materials. Initial results demonstrated that flame speed in open channels can eclipse 1 km/s and is comparable to on-chip porous silicon. This study further investigates flame speed characterization of these particles with various oxidizers, and explores mixture of this material with various binders for additive manufacturing applications. FTIR, EDS, TEM, SEM, high speed imaging, bomb calorimetry have all been used to characterize the particles and/or energetic formulations.

2:30pm **C4-4 Investigating Transport Processes in Multilayer Films***, **David Adams**, M Abere, C Sobczak,* Sandia National Laboratories, USA

Metallic thin film multilayers that undergo rapid, self-propagating formation reactions are of interest for several applications including advanced joining technology. The development and optimization of new materials for these applications requires a detailed understanding of mass transport, chemical reactions, heat release and thermal transport processes. With this presentation, we focus on the thermal properties of produced multilayers. Thermoreflectance techniques have been used to characterize the thermal conductivity of different Pt/Al, Co/Al and Ni/Al multilayers. The bilayer thickness dependence of cross-plane thermal conductivity has been determined for various multilayers. The results are examined in terms of conductivity through the reactant layers and the role of interfaces. The interfacial structure and composition of each system has been mapped by cross section transmission electron microscopy. The measured properties are compared with estimates derived from analytical modeling of self-propagating formation reactions. The model developed by Mann et al. (J. Appl. Phys. 1997) to predict how measured flame speeds vary with multilayer design is used to estimate the thermal and mass transport characteristics. This analytical model accounts for reactant layer thicknesses, compositional profiles near interfaces, flame temperatures, measured heats of reaction, measured activation energies, and adiabatic temperatures.

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2:50pm **C4-5 Analytical Modelling of Propagation Velocity in Non-stoichiometric and Impact Compressed Nanolaminates***, **Michael Abere**, D Adams,* Sandia National Laboratories, USA

The ignition of sputter deposited bimetallic nanolaminate films results in rapid, self-propagating reactions. Analytical models of the measured propagation velocities have been typically performed using a framework developed by Mann et al. (J. Appl. Phys. 1997). This work seeks to expand upon this model to handle bimetal systems such as Al/Pt in which the lateral and transverse thermal conductivity are highly anisotropic. A thermal circuit model is thus employed that is shown to hold for both equimolar and non-stoichiometric compositions of Al/Pt. Furthermore, this work utilizes cross-sectional scanning transmission electron microscope energy-dispersive X-ray spectroscopy data to calculate the Fourier coefficients in the Mann et al. model from the physical composition profile in the intermixed region. The same framework can also be applied to determine the magnitude of plastic deformation necessary after laser flyer impact to produce observed propagation velocities as much as a factor of two above the steady state velocity of NiV/Al within the impacted zone.

3:10pm **C4-6 On the Fly Mixing and 3D Printing of Al/CuO Thermite for Controlling Reactivity***, **Alexandra Golobic**, M Durban,* Lawrence Livermore National Laboratory, USA*; E Duoss,* Lawrence Livermore National Laboratory, USA, US*; A Gash, K Sullivan,* Lawrence Livermore National Laboratory, USA

The ability to spatially control the behavior of reactive materials *within* a part is now a reality with advances in 3D printing. This vastly opens up the design space for rapidly deflagrating materials, such as pyrotechnics or thermites, to yield a precise property or dynamic performance. In order achieve this goal, a mixing print head was used to mix an aluminum and a copper oxide ink on the fly. The mixing and printing parameters were first investigated for a stoichiometric mix of fuel and oxidizer to determine at what point the material can be assumed well-mixed. The equivalence ratio was then changed, and the critical mixing parameters established. The reactivity was characterized by printing a strip of material, then initiating the thermite and measuring the propagation velocity with a high-speed camera. Once the velocity reached a plateau, we considered the system well mixed. 3D printing was then used to make parts where the local stoichiometry, which corresponds to performance, is spatially varied. Collective effects of having incorporated features with differing reactivates were investigated.

3:30pm **C4-7 Tin-based Composites Combined with Reduced Graphene Oxide via a Simple Chemical Treatment as Anode Material for Rechargeable Lithium Ion Batteries***, **Yi-Zhu Wu**,* National Cheng Kung University, Taiwan*; C Chang,* National University of Tainan, Taiwan*; S Brahma, J Huang,* National Cheng Kung University, Taiwan

We successfully synthesize the reduced graphene oxide/SnO_x (RGO/SnO_x) composites via a one-step chemical treatment with low cost and low toxicity at room temperature. In this procedure, we use the $Sn(BF_4)_2$ as the precursor and $NaBH_4$ as the reducing agent to deposit the tin onto reduced graphene oxide and utilize the composite as anode material for lithium ion batteries. With different concentration of reducing agent, we can control different reduction degree of composites. This study shows that reductant concentration significantly affect the density and agglomeration of nanoparticles over the GO sheets. The average size of the nanoparticles in the composites is approximately 5 nm. The observed electrochemical performance of RGO/SnO_x composite shows improved capacity (937.9 mAh/g for first cycle discharge) and good cycling ability (824.0mAh/g with 88% retention after 50 cycles.).

3:50pm **C4-8 Additive Manufacturing of a Composite Solid Propellant with High Solids Loadings***, **Monique McClain**, I Gunduz, S Son,* Purdue University, USA

Solid propellant performance is strongly dependent on the manufacturing process. The traditional method of casting propellant limits the ability to locally vary geometry and reactivity throughout the grain and could lead to the creation of defects. Additive manufacturing (AM) has been effectively demonstrated as an alternative manufacturing process for complex hybrid propellant grains. However, methods such as jet printing, stereolithography, and fuse deposition modeling are limited by the materials that can be printed. Conventional printable materials are less reactive than baseline fuels, such as hydroxyl-terminated polybutadiene (HTPB), and high solids loadings have not been achieved, rendering the printing of high performing solid propellants unobtainable. In this work, an AM method developed in our lab was used to print ammonium perchlorate (AP) composite propellant strands at 85% solids loading. The viscosities of AP propellant mixtures were characterized to quantify printing parameters and the integrity of the samples were investigated with X-ray tomography scans. The printed AP propellant strands were burned at high pressure to determine the burning rate and were compared to cast samples with the same formulation. It was demonstrated that AM could be used to manufacture solid propellants at a solids loading comparable to current industry standards.

4:10pm **C4-9 Manufacturing and Characterization of Nanocomposite WC-based Powders***, **Abdulsalam Alhazza,** L Al-Hajji, S El-Eskandarani, A Al-Rowayyeh,* Kuwait Institute for Scientific Research, Kuwait

In the present work, the structural, mechanical, chemical, and morphological characterizations of the synthesized powders and their consolidated buttons was investigated. The synthesized powders are mechanically-induced solid state mixing or synthesizing of nanocomposite WC-Co-metal oxide (Al_2O_3, MgO, SiO_2, and ZrO_2) s uperhard material powders.

During the consolidation and manufacturing process, the nanocrystalline characteristic of the nanocomposite should be noticed and maintained to take advantage of the unique properties of the synthesized nanocomposites.

The consolidation of the nanocomposite powders will lead to the manufacturing full dense buttons with a very high hardness, fracture toughness, and wear resistance by synthesizing a nanosized powders and advent of fast sintering techniques.

4:30pm **C4-10 Ternary Reactive Ru/Al/X Multilayers - The Effect of Stacking Sequence on Ignition, Propagation and Microstructure Evolution***, **Christoph Pauly,*** Saarland University, Germany*; K Woll,* Karlsruhe Institute of Technology (KIT), Germany*; I Gallino,* Saarland University, Germany*; M Stüber,* Karlsruhe Institute of Technology (KIT), Germany*; F Mücklch,* Saarland University, Germany **INVITED**

To date, self-propagating reactions in PVD multilayers have been extensively studied regarding their underlying mechanisms and applications. Adjusting the reaction behavior to meet the demands of an application requires a fundamental understanding of the mechanisms and transformations on the micro- and nanoscale. Interfacial reactions are found to play a key role in determining reaction parameters such as front propagation, heat release over time and ignition behavior. The majority of studies use binary samples consisting of elemental or alloyed layers where the bilayer thickness is the main design parameter while the material combination at the interface remains unchanged. By introducing a third kind of layers, the stacking sequence becomes an additional design parameter allowing us to define type and density of the interfaces.

In this study, we designed ternary reactive multilayers based on Ru/Al by partially substituting either Ru or Al for selected elements which allows us to retain the B2-structure of the product phase. The system Ru/Al shows a heat of formation and propagation velocity comparable to that of Ni/Al, however, its temperature of reaction and ignition are higher. We present how stacking sequence and ternary additions affect the properties of the self-propagating reaction. The role of interfacial solid state reactions on ignition is discussed and how this can be used to modify ignition temperatures. Strong effects of composition and stacking sequence on net propagation velocity are observed and discussed with the help of microstructural analysis of quenched reaction fronts.

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