PhD Dissertation Titles & Abstracts for 2017 Graduates

Inigo Anza

Advisor: Prof. Makhlouf Makhlouf

Synthesis of Aluminum-Titanium Carbide Composites by the Rotating Impeller Gas-Liquid In-situ Method

Abstract:

The next generation of aluminum automotive engines will have to operate at temperatures approaching 300°C. Traditional aluminum alloys cannot perform at these temperatures, but aluminum alloys reinforced with fine particles can. The objective of this research is to develop a process to synthesize Al-TiC composites by the Rotating Impeller Gas-Liquid In-situ method. This method relies on injecting methane into molten aluminum that has been prealloyed with titanium. The gas is introduced by means of a rotating impeller into the molten alloy, and under the correct conditions of temperature, gas flow, and rotation speed, it reacts preferentially with titanium to form titanium carbide particles. The design of the apparatus, the multi-physics phenomena underlying the mechanism responsible for particle formation, and the operation window for the process are first elucidated, then a parametric study that leads to the synthesis of TiC reinforced aluminum is described. Finally, potential technical obstacles that may stand in the way of commercializing the process are discussed and ways to overcome them are proposed.

Meinan He

Prof. Yan Wang

High Voltage Electrolyte Based on Fluorinated Compounds for High Energy Li-ion Chemistry

Abstract:

Lithium ion batteries have dominated the portable electronics market. They have the potential to dominate large-scale battery applications including hybrid and electric vehicles, as well as grid storage, because of their high energy and power densities. It is well known that conventional electrolytes show poor anodic stabilities above 4.5 V versus Li/Li^{+}. As a result, high voltage electrolytes are essential for the development of next generation lithium ion batteries. Both fluorinated electrolytes and additives can be introduced in to the electrolyte system. In this work, fluorinated electrolytes were introduced into graphite-$LiNi_{0.5}Mn_{0.3}Co_{0.2}O_2$ (operated between 3.0 - 4.6 V) and graphite- $LiNi_{0.5}Mn_{1.5}O_4$ (operated between 3.5 - 4.9 V) full cell systems. The baseline electrolyte for all cells (referred to as Gen2) was composed of 1.2M $LiPF_6$ dissolved in a mixture of EC and EMC (3:7 in weight ratio). After a series of electrochemical tests, compared to the baseline electrolyte, the fluorinated electrolytes displayed significantly enhanced performance under both high cut off voltage and high temperature (55 °C). The post test analysis results showed that the cycled electrode can not only reach a much more stable interface but also can overcome the crystal structure change after long term cycling when the fluorinated electrolyte system was used. In addition to changing the solvent, a series of additives were designed, synthesized and evaluated for high-voltage Li-ion battery cells using a Ni-rich layered cathode materials $LiNi_{0.5}Co_{0.2}Mn_{0.3}O_2$ (NCM523). The repeated charge/discharge cycling for NCM523/graphite full cells using Gen2 with 1 wt % of these additives as electrolytes was performed. Electrochemical performance testing and post analysis result demonstrate that our as selected or designed cathode additives can passivate the cathode and prevent the cathode from side reactions. The methodology developed could be fundamental in the design and investigation of better electrolytes for the next generation lithium ion batteries.

Baillie McNally

Prof. Richard Sisson, Jr.

Through-Process Modeling of Aluminum Alloys for Cold Spray: Model Development and Experimental Characterization

Abstract:

The cold spray process is a cost effective process for repairing damaged parts or creating structural bulk materials for military aircraft that require high maneuverability, durability, ballistic protection, and energy efficiency. This process can be made even more robust with a predictive tool that would tailor the material and processing parameters to a variety of repair applications. A through-process model that includes powder production, powder processing, the cold spray particle impact, and post-processing would benefit the current trial and error efforts immensely and would aid in the search for an optimal cold spray alloy for different applications. The powder production stage addresses the microstructure, phases and strength that result from the gas atomization process. The powder processing stage takes into account any microstructural effects from heat treating or degassing the powder before it is cold sprayed. The particle impact stage includes a finite element model that simulates the temperature generation and strain that occurs during cold spray. An additive strength model, which is applied to the powder and used as an input into the impact model, determines the contributions of solid solution, microstructural, and precipitation strengthening and is a function of particle diameter, and time and temperature of powder processing. The important parameters that are experimentally characterized to verify and enhance the described models are grain size, phase morphology and fraction, and nanohardness. Characterization techniques such as optical, scanning and transmission electron microscopy, focused-ion beam, x-ray diffraction, and nanoindentation are used to verify the various stages of the through-process model for aluminum alloys 6061 and 5056.

Yinjie Cen

Prof. Jianyu Liang

Si/C Nanocomposites for Li-Ion Battery Anode

Abstract:

The demand for high performance Lithium-ion batteries (LIBs) is increasing due to widespread use of portable devices and electric vehicles. Silicon (Si) is one of the most attractive candidate anode materials for the next generation LIBs because of its high theoretical capacity (3,578 mAh/g) and low operation potential (~0.4 V vs Li+ /Li). However, the high volume change (>300%) during Lithium ion insertion/extraction leads to poor cycle life. The goal of this work is to improve the electrochemical performance of Si/C composite anode in LIBs. Two strategies have been employed: to explore spatial arrangement in micro-sized Si and to use Si/graphene nanocomposites. A unique branched microsized Si with carbon coating was made and demonstrated promising electrochemical performance with a high active material loading ratio of 2 mg/cm^2, large initial discharge capacity of 3,153 mAh/g and good capacity retention of 1,133 mAh/g at the 100th cycle at 1/4C current rate. Exploring the spatial structure of microsized Si with its advantages of low cost, easy dispersion, and immediate compatibility with the prevailing electrode manufacturing technology, may indicate a practical approach for high energy density, large-scale Si anode manufacturing. For Si/Graphene nanocomposites, the impact of particle size, surface treatment and graphene quality were investigated. It was found that the electrochemical performance of Si/Graphene anode was improved by surface treatment and use of graphene with large surface area and high defect density. The 100 nm Si/Graphene nanocomposites presented the initial capacity of 2,737 mAh/g and good cycling performance with a capacity of 1,563 mAh/g after 100 cycles at 1/2C current rate. The findings provided helpful insights for design of different types of graphene nanocomposite anodes.

Aaron Birt

Prof. Diran Apelian

Materials & Machines: Simplifying the Mosaic of modern Manufacturing

Abstract:

Manufacturing in modern society has taken on a different role than in previous generations. Today's manufacturing processes involve many different physical phenomenon working in concert to produce the best possible material properties. It is the role of the materials engineer to evaluate, develop, and optimize applications for the successful commercialization of any potential application. Laser-assisted cold spray (LACS) is a solid state manufacturing process relying on the impact of supersonic particles onto a laser heated surface to create coatings and near net structures. A process such as this that involves thermodynamics, fluid dynamics, diffusion, localized melting, deformation, recrystallization, and heat transfer is the perfect target for developing a data science framework for enabling rapid application development with the purpose of commercializing such a complex technology in a much shorter timescale than was previously possible. A general framework for such an approach will be discussed, followed by the execution of the framework for LACS. Results from the development of such a materials engineering model will be discussed as they relate to the methods used, the effectiveness of the final fitted model, and the application of such a model to so solving modern materials engineering challenges.

Carl Soderhjelm

Prof. Diran Apelian

Multi-Material Metal Casting: Metallurgically Bonding of Aluminum to Ferrous Inserts

Abstract:

Properties of cast aluminum components can be improved by strategically placing ferrous inserts to locally improve properties such as wear resistance and stiffness. A cost-effective production method is to cast-in the insert using the solidification of the molten aluminum as a joining method. Metallugically bonding between the metals could potentially improve both load and heat transfer across the interface. The metallurgical bond between the steel and the aluminum has to be strong enough to withstand stresses related to solidification, residual stresses, thermal expansion stresses, and all other stresses coupled with the use of the component. Formation of a continuous defect free bond is inhibited by the wetting behavior of aluminum and is governed by a diffusion process which requires both energy and time. Due to the diffusional nature of the bond growth in combination with post manufacturing heat treatments defects such as Kirkendall voids can form.

The effect of aluminum alloying elements during liquid-solid bond formation in regards to microstructural changes and growth kinetics has been described. A timeframe for defect formation during heat treatments as well as microstructural changes has been established. The effect of low melting point coatings (zinc and tin) on the nucleation of the metallurgical bond has been studied as well the use of a titanium coating for microstructural modification. A set of guidelines for successful metallurgical bonding during multi-material metal casting has also been constructed

Anthony Spangenberger, III

Prof. Diana Lados

Engineering of Light Metals for Dynamic Properties and Fatigue Performance

Abstract:

Fatigue crack growth-based design is a significant modern engineering consideration, and its implementation requires accurate characterization and understanding of crack propagation mechanisms. To address this need, light structural aluminum alloys representing multiple microstructural failure mechanisms have been created through processing and chemistry means in order to systematically investigate the individual and combined effects of the materials' characteristic microstructural features on fatigue crack growth.

Crack-microstructure interactions and failure mode transitions were investigated and have been identified with respect to the controlling features (eutectic Si morphology/distribution and grain structure) by fractographic and novel techniques. Complementary to this work, an original methodology has been developed to predict microstructurally small fatigue crack growth data in order to minimize extensive and costly materials testing. A computational framework has been further developed for microstructure-specific fatigue crack growth and with phase property data calculated from novel microhardness indentation experiments. The net effect of this project will be to provide a methodology and toolset for design with enhanced fatigue crack growth resistance, life predictions, and material / process optimization.