# Thursday Afternoon, May 23, 2019

# Fundamentals and Technology of Multifunctional Materials and Devices

#### Room Pacific Salon 3 - Session C4-ThA

#### Fundamentals of Metallurgy in Thin Films and Coatings

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

1:40pm C4-ThA-2 Analytical Modelling of Propagation Velocity in Electron Transparent Nanolaminates, *Michael Abere*, Sandia National Laboratories, USA; *G Egan*, Lawrence Livermore National Laboratory, USA; *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 electron transparent Co/Al samples for experiments in dynamic TEM. This work utilizes a three resistor thermal circuit model to account for thermal conductivity in the intermixed zone that is an order of magnitude less than that predicted by rule of mixtures. Also, 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 effect of radiation loss for 150 nm thick foils is calculated as a perturbation to the difference in the heat of reaction measured in calorimetry and the adiabatic heat of product formation. Finally, the model considers two independent activation energies for when the reaction proceeds via co-melted reactants versus solid Co dissolution into molten Al.

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(LDRD) program. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under Contract No. DE-NA0003525. This work describes objective technical results and analysis. Any subjective views or opinions that might be expressed in the paper do not necessarily represent the views of the U.S.

Department of Energy or the U.S. Government.

## 2:40pm C4-ThA-5 Twin-Wire Arc Coatings for Repair of Structural Components, *C Jasien, Nicole Wagner*, Cal Poly Pomona, USA

There has been a growing interest in additive manufacturing technologies for the repair of metallic structural components. Among the proposed techniques, twin-wire arc plasma spraying offers the advantage of providing high deposition and growth rate capabilities, coupled with process robustness and versatility, which are always desirable in real-life applications. In addition to these considerations, the fundamental materials science of these plasma-sprayed coatings is surprisingly still under-explored. Nanostructured depositions and coatings should be achievable with this additive technique given its high temperature and fast quenching rate. Motivated by these considerations, we have performed a study on the deposition of metallic coatings on steel substrates using an Oerlikon Metco FlexiArc 300 twin-wire arc plasma spraying system. We used 1.6mm diameter stainless steel wires and compressed air as a carrier gas. The process conditions that were varied include power, standoff distance and coating thickness. Dense coatings, approximately 150 micrometers thick, were achievable at the highest electrical input power of 10 kW within a few seconds of deposition time. Structural and morphological characterization has been performed using scanning electron microscopy (SEM) and energy dispersive x-ray spectroscopy (EDS). We have found that substrate temperature has a significant influence on the adhesion layer between the substrate and the coating.

3:00pm C4-ThA-6 Unstable Propagating Reactions in Sputter-Deposited Nanolaminates, *David Adams*, *M Abere*, Sandia National Laboratories, USA Reactive metal multilayers are a form of energetic material that continue to attract attention for various applications. Generally composed of two layered reactants, these heterogeneous solids can be stimulated at a point or in bulk to initiate internal, self-sustained chemical reactions that give off heat and light. Their reactions are characterized by propagating high temperature wavefronts, little or no gas emission, and rapid local heating

rates of ~106 K/s. Reactions often propagate in a stable manner characterized by a uniform propagation speed and smooth wavefront morphology. Other less reactive forms exhibit unstable reactions characterized by stalled wavefronts, spatially non-uniform temperatures, and variable propagation speeds. Unfortunately, unstable reaction modes are poorly understood, thus limiting the use of reactive multilayers in emerging applications. In order to better understand the various behaviors of reactive multilayers, we have investigated how surrounding gaseous environment affects wavefront stability. Rare-earth / transition metal multilayers (e.g., Sc/Ag) of different periodicity were deposited by DC magnetron sputtering and tested as freestanding foils in different environments. Their reaction in 1e-3 Torr vacuum demonstrates inherent unstable intermetallic reaction fronts. Reactions in air are complicated by oxidation of the rare earth metal species which produces metal oxide and residual elemental metal. A separate oxidation wavefront trails the intermetallic reaction wavefront when reacted in air. In some cases, oxidation occurs long after the passage of the intermetallic reaction and there is little effect on the intermetallic reaction dynamics. However, largeperiod (low speed) multilayers show evidence for interference between intermetallic and trailing oxidation reaction waves. Prompt oxidation after the passage of the slow intermetallic reaction wave leads to a complex oscillatory behavior. The high exothermicity oxidation reaction repeatedly transitions the intermetallic front from an unstable mode to a stable form, while boosting its net velocity.

This work was supported by a Sandia Laboratory Directed Research and Development (LDRD) program. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

3:20pm C4-ThA-7 Synthesis of Reactive Ni-Al Composites Using High Pressure Torsion, O Renk, Austrian Academy of Sciences, Austria; M Tkadletz, N Kostoglou, Montanuniversität Leoben, Austria; I Gunduz, Naval Postgraduate School, USA; C Doumanidis, Nazarbayev University, Astana, Kazakhstan; R Pippan, Austrian Academy of Sciences, Austria; C Mitterer, Montanuniversität Leoben, Austria; Claus Rebholz, University of Cyprus, Cyprus

Mechanical mixing methods provide a bottom-up scalable route for fabricating nanostructured bulk materials. These include high energy ball milling (HEBM) used in metal-based reactive systems such as Nickel-Aluminum that can yield high performance NiAl and Ni<sub>3</sub>Al intermetallic alloys upon combustion synthesis or used for in-situ welding with the heat generated from the exothermic reactions. The drawback of HEBM is the final product form, which consists of fine hardened powders that need to be processed further to form a dense part. This study investigates an alternative route, high pressure torsion (HPT), which applies a combination of large normal and shear stresses to a powder mixture in a die to vield nanostructured materials. HPT was used for fabricating consolidated reactive pellets of Ni-Al with microstructures comparable to HEBM and magnetron sputtering. The results show that materials undergoing HPT beyond 5 full rotations at processing temperatures of up to 473 K are highly reactive and can be ignited below the AI melting point, yielding a product phase of NiAl with residual Ni<sub>2</sub>Al<sub>3</sub> and Ni<sub>3</sub>Al, while reaching very high reaction temperatures near 1900 K.

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