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Imre J. Rudas

Applied Mathematics and Materials

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Tiecheng Xia
Stevo Stevic
Lucas Jodar
Noemi Wolanski
Zhenya Yan
Juan Carlos Cortes Lopez
Wei-Shih Du
Kailash C. Patidar
Hossein Jafari
Abdel-Maksoud A Soliman
Janusz Brzdek
Marius Marcu
Eleazar Jimenez Serrano
Ahmet Arslan
Kemal Tutuncu
Humar Kahramanli
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Hongjun Liu
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Snezhana Georgieva Gocheva-Ilieva
Elena Scutelnicu
Dana Anderson
Muhammet Koksal
Md. Shamim Akhter
Sk. Sarif Hassan
Emmanuel Lopez-Neri
Vassos Vassiliou
Yuqing Zhou
Gabriella Bognar
Zanariah Abdul Majid
U. C. Jha
Anca Croitoru
Hamideh Eskandari
Bhagwati Prasad
Ibrahim Canak

Table of Contents

ISBN: 978-1-61804-347-4

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Plenary Lecture 1

A Hybrid Deterministic/Probabilistic Model for Metal Vapor Transport in Physical Vapor Deposition (PVD) Process

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Abstract: Electron-beam physical vapor deposition (EB-PVD) is an established technology for producing unique material coatings for a variety of applications. In this process, a pre-selected metal ingot (the target) is vaporized in an evacuated chamber with a high power electron beam. The metal vapor flows across the high-vacuum chamber and is deposited on the component of interest (substrate). The process of vaporization and transport of metal vapors in near-vacuum involves a dense region just above the target, which quickly expands and becomes rarefied on route to the substrate. The goal of this research is to better understand the PVD vapor transport process by determining the most appropriate fluidic model to design PVD coating manufacturing. The vapor transport process is characterized by a wide range of values of the Knudsen number, Kn, which is defined as a ratio of the mean free path of atoms or molecules to a characteristic dimension, such as the target diameter (Kn = ?/D). The Knudsen number increases from a very low value on the order of 10-6 just above the evaporating target surface (signifying a highly dense, continuum regime), to a value of around 10 near the substrate (signifying a highly rarefied, almost free molecular regime). Any attempt to create an optimal mathematical model of this process requires successful descriptions of each of these regions. The continuum regime (Kn < 0.01) is best described by Computational Fluid Dynamics (CFD), the deterministic solution of the Navier-Stokes equations. Whereas, the transitional and rarefied regimes (around 0.01 < Kn < 10) require the application of the particle tracking probabilistic Direct Simulation Monte Carlo (DSMC) technique. In the modeling of the EB-PVD process, both these techniques are needed due the extreme density gradient and highly non-ideal nature of the metal vapor.
In this research, a hybrid CFD-DSMC solver is developed in OpenFOAM software to model the vapor transport process by Navier-Stokes and DSMC equations, and then the two regions are patched through a novel boundary condition. The velocity and temperature information is sent one-way from the CFD region to the DSMC region to appropriately define the energy states of the particles created at the boundary, and either pressure or density is interpolated between the regions to create the appropriate number of particles at the boundary. A comparison to experimental data was performed to determine if the unique physics of each fluidic model have a substantial effect on the expected deposition profile. The results showed the hybrid solver yields the widest range of reasonable results over either the Navier-Stokes or the DSMC solutions. Thus, in conclusion, the recommended fluidic model for PVD vapor transport is a hybrid CFD-DSMC solver using some form of a domain decomposition. Results also show that extreme care must be taken when modeling EB-PVD processes for design purposes, as the incorrect choice of flow regime will yield inaccurate inlet criteria.

Brief Biography of the Speaker: Professor Kulkarni joined as a faculty member in the Department of Mechanical Engineering at The Pennsylvania State University in 1980 after completing Sc. M. and Ph. D. degrees from Brown University, Providence, Rhode Island. His academic areas of interest are, engineering education, energy, materials processing, heat transfer, computational fluid mechanics, combustion, and professional ethics. Currently he is active in two areas- (i) in Materials Science, he has been conducting research on Electron Beam Physical Vapor Deposition (EB-PVD) and Field Assisted Sintering Technology (FAST), and (ii) in Energy area, he has been working on developing an optimization tool for hybrid power plants to be used in rural/remote areas. At Penn State, Dr. Kulkarni has taught courses in Thermodynamics, Indoor Air Quality Engineering, Propulsion and Power Systems, and Measurements and Instrumentation. He also has served as the Professor-in-charge of Mechanical Engineering Graduate Program for eight years, project director for an NSF-funded Environmentally Conscious Manufacturing Graduate Research Traineeship program at Penn State, and as an elected Faculty Senator and Graduate Council member at Penn State University, among other positions. Recently, Dr. Kulkarni was awarded US – Norway Fulbright Scholarship by the U. S. government for working on Indoor and Outdoor Fugitive Emissions in the Materials Processing Industry. He has had international collaborative activities with Australia, China, Germany, India, Japan, Norway, and former USSR.

Plenary Lecture 2

Perovskites: Novel Materials for Stable and High-Efficiency Solar Cells

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Abstract: Organic-inorganic perovskites, such as CH3NH3 Pb X3 (X = I- or Br-), are quickly leading to research activities in new materials for cost-effective and high-efficiency photovoltaic technologies. Since the first demonstration from Kojima and co-workers in 2009, several perovskite-based solar cells have been reported and certified with rapidly improving power conversion efficiency. Recent reports demonstrate that perovskites can compete with the most efficient inorganic materials, while they still allow processing from solution as potential advantage to deliver a cost-effective solar technology. I will discuss the most recent advances to prepare stable and high-efficiency perovskite solar cells. The current most efficient perovskite solar cells employ small molecule or polymeric organic semiconductors as hole transporting layer within the device architecture. I will show that the hole transporter has a strong impact on the device lifetime and I will report new organic semiconductors that allow to prepare more stable and high-efficiency perovskite solar cells. Then, I will show that electronic trap states at the organic-inorganic interface between the perovskite crystal surface and the hole transporting layer generate charge accumulation and consequent recombination losses. I will demonstrate that under-coordinated iodine ions within the perovskite structure are responsible and make use of supramolecular halogen bond complexation to successfully passivate these sites and thus improve the power conversion efficiency.

Brief Biography of the Speaker: I am currently a Marie Curie Research Fellow at École Polytechnique Fédérale de Lausanne and I am acting as Research Group Leader at Adolphe Merkle Institute, University of Fribourg in Switzerland. After completing my PhD training at Politecnico di Milano in Italy, I spent 4 years as Postdoctoral Researcher at the University of Oxford and the University of Cambridge in the United Kingdom. My research interests are in hybrid organic-inorganic materials for optoelectronics.

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Authors Index

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