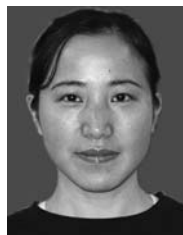


## Meet Our New Colleagues

This column presents selected currently graduating Ph.D. students in the thermal spray field from around the world. Students planning to graduate in the area of thermal spray within next 3-6 months are encouraged to submit a short description (1-2 pages, preferably as Word document) of the projects they performed during their studies to Jan Ilavsky, JTST Associate Editor, address: Argonne National Laboratory, Advanced Photon Source, 9700 S. Cass Ave., Argonne, IL, 60439; e-mail: JTST.ilavsky@aps.anl.gov. After limited review and corrections and with agreement of the student's thesis advisor, selected submissions will be published in the upcoming issues of JTST.

### Prediction of the Microstructure of Plasma Spray Coating Deposits

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Minxia Xue

#### Background and Motivation

Since thermal spraying process allows use of a wide variety of materials that melt without decomposing to make a coating, thermal spray coating technologies are widely used in many sectors

to protect surfaces against heat, wear, or corrosion. There are various thermal spraying technologies that may produce coatings with different microstructures. Even the same spraying technology, depending on operating parameters, may result in different coating microstructures.

Since the operational cost of thermal spraying is relatively high, developing new coatings through large numbers of experiments is not economical. A computer model capable of predicting the coating properties as a function of process parameters will greatly reduce the development time and cost. It can also improve and optimize the design of spraying guns and tailor coating properties to meet the needs of individual applications.

The objective of this research program was to extend and improve a stochastic model of thermal spray coating formation and accurately predict coating properties as a function of process parameters.

#### Methodology

The model assigns impact properties to molten droplets landing on the substrate by generating random values of process parameters, assuming that these properties follow normal distributions with user-specified means and standard deviations. By expressing particle impacting velocity as a function of particle size and temperature, the degree of freedom in the simulation can be reduced. The size of the splat formed by an impacting particle with known size, temperature, and velocity on a solid surface are calculated using a simple analytical expression proposed by Aziz and Chandra (Ref 1).

Based on experimental results, and some simulations of sequential droplet impact using a three-dimensional model (Ref 2) four possible scenarios for the second splat shape formed by two-droplet interactions have been developed. The shape of the second splat depends on the offset distance between the two interacted droplets.

Porosity is defined as the fraction of the total coating volume occupied by voids. To date, two possible sources of porosity have been considered: curling up at the edges of splats due to thermal stresses and incomplete filling of interstices during deposition (Ref 3).

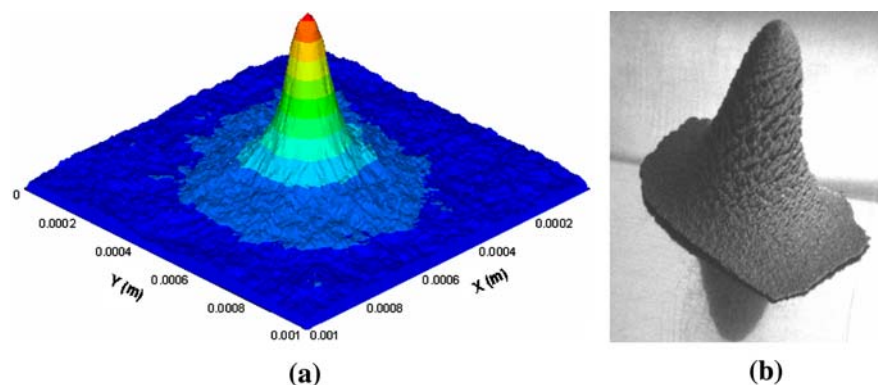
The spraying gun can be user-specified as a moving gun with defined motion speed or as a stationary gun with defined position. When a specific number of passages have been reached, or a specific amount of coating mass/time has been consumed, the deposition process will stop and the coating properties will be calculated.

A three-dimensional Cartesian grid is used to define the computational domain and to track the shape and position of the coating surface. The structure of the coating is defined using the variable known as volume-of-fluid ( $f$ ) (Ref 1) defined as the fraction of a cell volume occupied by the splats.

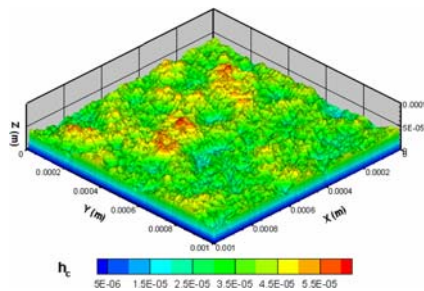
#### Major Results

The deposition of yttria-stabilized zirconia (YSZ) particles on a stainless steel surface is taken as an example to present the coating simulation results. The first result is from a simulation in which a stationary gun was standing at a distance of 50 mm from the substrate, with a powder mass flow rate of 0.13 g/s. The gun was positioned at the center of the substrate. Figure 1(a) shows the coating profile after the gun sprayed for 10 ms. The Gaussian shape of the profile is very similar to those observed experimentally in Fig. 1(b).

In the next simulation, the gun moved at 0.4 m/s to-and from along the  $x$ -direction for four passages. The simulated coating profile is shown in Fig. 2. Since the gun-disperse angle is relatively large, the particles were deposited evenly and



**Fig. 1** (a) Simulation image of the coating surface formed by YSZ particles deposited on a  $1 \times 1 \text{ mm}^2$  stainless steel substrate with a stationary gun positioned at the substrate center. (b) Typical experimental topology of coating produced by a stationary gun



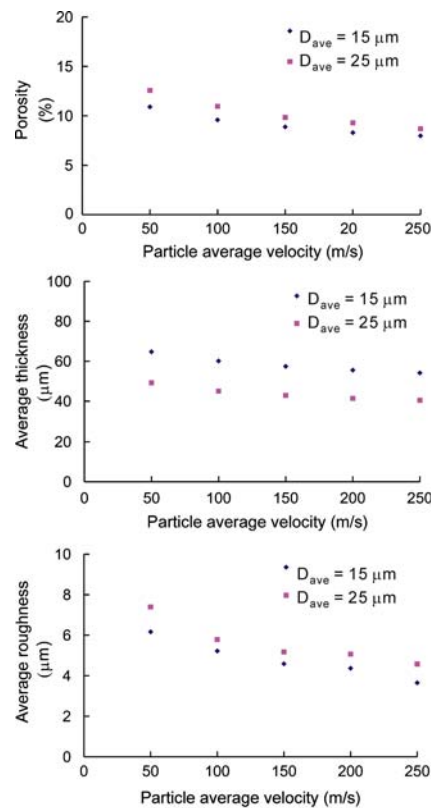
**Fig. 2** Simulation images of the coating microstructures formed by YSZ particles impacting on a  $1 \times 1 \text{ mm}^2$  stainless steel substrate with constant gun movement

formed a flat coating with some surface roughness.

To examine the effect of particle size and velocity on the coating properties, the deposition of two different sizes of particles with impact velocity between 50 and  $\sim 250 \text{ m/s}$  is simulated. The average diameters of the particles are 15 and  $25 \mu\text{m}$ . Figure 3 shows the values of porosity, average thickness, and roughness with particle size and velocity. All the coating properties, porosity, average thickness, and roughness, are found to decrease with impact velocity. Figure 3 also demonstrates that a coating formed by larger particles with  $25 \mu\text{m}$  average diameter has greater porosity and average roughness than that formed by smaller particles with  $15 \mu\text{m}$  average diameter. This agrees well with experimental results. Also, it is the first time that we can correctly predict the relation between coating properties and particle size.

## References

1. S.D. Aziz and S. Chandra, Impact, Recoil and Splashing of Molten



**Fig. 3** Variations of coating porosity, average thickness, and roughness with particle size and velocity

1. Metal Droplet, *Int. J. Heat Mass Transfer*, 2000, **43**(16), p 2841-2857
2. R. Ghafouri-Azar, J. Mostaghimi, S. Chandra, and M. Charmchi, A Stochastic Model to Simulate the Formation of a Thermal Spray Coating, *J. Therm. Spray Technol.*, 2003, **12**(1), p 53-69
3. M. Xue, S. Chandra, and J. Mostaghimi, Investigation of Splat Curling up in Thermal Spray Coat-

ings, *J. Therm. Spray Technol.*, 2006, **15**(4), p 531-536

## Author's Recent Publications

- M. Xue, Y. Heichal, S. Chandra, and J. Mostaghimi, Modeling the Impact of a Molten Metal Droplet on a Solid Surface Using Variable Interfacial Thermal Contact Resistance, *J. Mater. Sci.*, 2007, **42**(1), p 9-18
- A. McDonald, M. Xue, S. Chandra, J. Mostaghimi, and C. Moreau, Modeling Fragmentation of Plasma-Sprayed Particles Impacting on a Solid Surface at Room Temperature, *C.R. Acad. Sci.* (accepted Dec 2006)
- M. Xue, S. Chandra, and J. Mostaghimi, Investigation of Splat Curling up in Thermal Spray Coatings, *J. Therm. Spray Technol.*, 2006, **15**(4), p 531-536
- M. Xue, J. Mostaghimi, and S. Chandra, Numerical Simulation of Coating Deposition in a Thermal Spray Process, *Proc. 13th International Heat Transfer Conference*, August 13-18, 2006 (Sydney, Australia)
- M. Xue, J. Mostaghimi, and S. Chandra, Formation of Pores in Thermal Spray Coatings Due to Incomplete Filling of Voids under Solid Particles, *Proc. 2006 International Thermal Spray Conference*, May 15-17, 2006 (Seattle, WA).
- M. Xue, J. Mostaghimi, and S. Chandra, Prediction of Coating Microstructure, *Proc. 2004 International Thermal Spray Conference*, May 10-12, 2004 (Osaka, Japan)