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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, 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 JTST.

Integration of Three-Dimensional Simulations and Diagnostic Experiments in Plasma Spraying

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Abstract of Research

Hongbing Xiong

Xiong works on the theoretical investigation of plasma spray process and the further integration of simulations with diagnostic experiments. A three-dimensional computational fluid dynamics code (CFD) named LAVA-P-3D has been developed with cosupport from Idaho National Engineering and Environmental Laboratory (INEEL). Special efforts have been directed to examine the plasma jet perturbation induced by the carrier gas flow and the entrained multiple particles. The main advantages offered by computational treatments of highly complex plasma spray process is the ability to study the influence of individual variables, such as operating conditions and feedstock properties and therefore to build a database for the process map. Computational tools can also provide insights to the phenomena that are difficult to be measured directly, such as in-flight particle evaporation and oxidation.

Key Results of Research

- **Three-dimensional model of plasma jet.** The extended three-dimensional numerical code, LAVA-P-3D, is a greatly enhanced version of the state-of-art LAVA code that is originally obtained from INEEL. The plasma jet is treated as a multicomponent, turbulent, chemically reacting ideal gas with temperature-dependent properties. LAVA is a 2D program specially designed for plasma spray process. LAVA-P-3D improved the interaction between the carrier gas flow and the plasma jet, as well as the multiple particles behavior, using a three-dimensional cylindrical geometry.

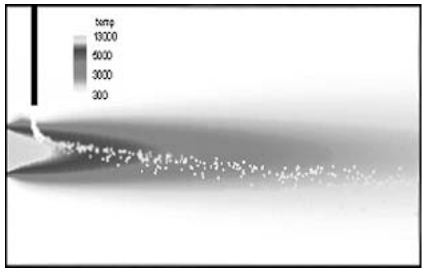

Fig. 1 3D numerical simulations of the thermal spray process. Contours depict the gas temperature while particle colors indicate melt fraction; blue is fully melted. (See Cover Photo for full color version of this figure)

- **Particle melting, resolidification, evaporation, and oxidation.** Particle melting and resolidification during in-flight are considered with nonuniform particle temperature. The particle evaporation is modeled as a mass and heat transport process either by heat transfer or vapor diffusion through the boundary. Three oxidation mechanisms are considered in molybdenum in-flight oxidation: diffusion in an oxide thin film, chemical reactions on the surface, and adsorption of oxidant diffused from the gas to the surface when the particle is melted.
- **Three-dimensional numerical study of plasma spray process.** Three-dimensional numerical simulation (Fig. 1) has been very helpful in improving the scientific understanding of the complex heat, momentum, and mass transport phenomena involved in thermal spray, as well as the process control and optimization. Computational results on molybdenum, NiCrAlY, and zirconium oxide particles in an argon-hydrogen DC plasma spray system have been obtained and discussed using our in-house-built 3D model. The temperature and melting formation of particles with different sizes along their trajectories are predicted (Fig. 2), as well as other particle parameters such as velocity, evaporation rate, and oxide content. The effects of gun power, flow rate of plasma gases, as well as carrier gas rate on the heating, acceleration, melting, evaporation, and oxidation of particles have also been discussed.

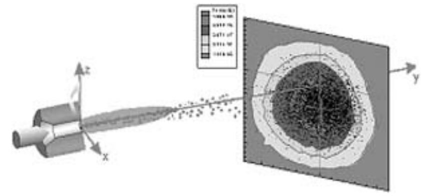

Fig. 2 Particle deposition on the substrate. Contours depict the average particle temperature.

- **Integration of simulations with experiments.** Further integration of simulations with diagnostic experiments have improved the understanding of plasma spray process, especially the particle melting during in-flight. A practical group parameter, melting index (M.I.) has been developed to characterize the melt fraction (Fig. 3), based on the experimentally measurable parameters such as particle size, velocity, and temperature. Melting index is based on the ratio of particle flight time and melting time. If melting index is larger than 1, it means the particle is well melted. As the interpretation of melting status, melting index has been used to optimize the spray distance, which allows optimal melting of particles and results in the good deposition efficiency (experiments conducted by L. Li, A. Vaidya, and T. Streibl).
- **RF (radio frequency) induction plasma spray and synthesis.** RF induction plasma spray, which emerges as a promising plasma technique in thin-film deposition and synthesis, has also been studied using an in-house-built two-dimensional program. The induction electromagnetic field and the ther-

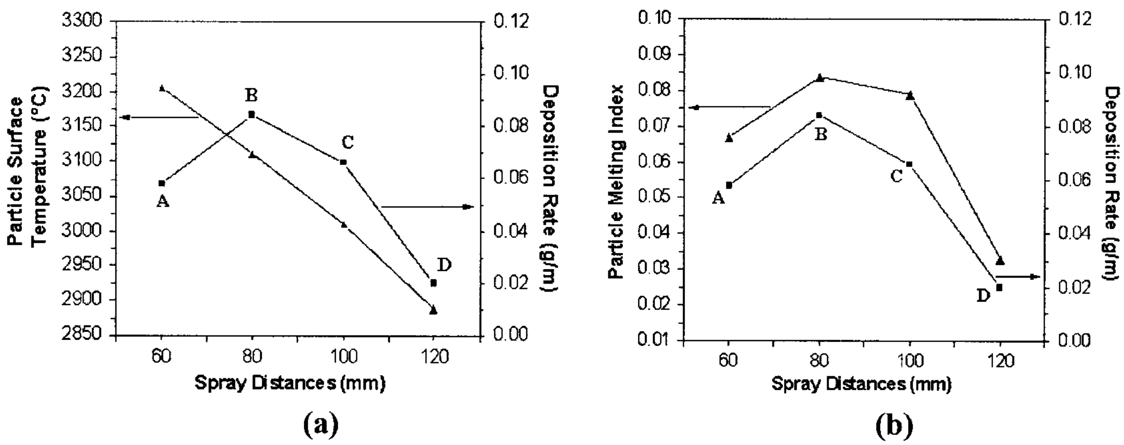

Fig. 3 The particle surface temperature decreases monotonically with the spray distance; while the deposition rate has a maximum value at distance of 8 cm. Therefore, the surface temperature is not a good indicator for deposition rate (**a**). On the contrary, a good correlation between the melting index and the splat deposition rate is observed as shown in (**b**).

mofluid field in the plasma flame have been investigated, as well as the injected particle behaviors under different operating conditions. Numerical results of the electromagnetic field were compared with the analytical solution and a good agreement has been achieved. Special attention has been directed to achieve good coupling between the electromagnetic field and the plasma field and how to inject the particles properly.

Publications:

- H.B. Xiong, L.L. Zheng, S. Sampath, and J.R. Fincke: "Melting/Oxidation Behavior of In-flight Particles in Plasma Spray Processes," International Mechanical Engineering Congress and Exposition (New Orleans, LA), 2002.
- H.B. Xiong, L.L. Zheng, S. Sampath, J.R. Fincke, and R.L. Williamson, "Three-Dimensional Simulation of Plasma Spray Jet," ASME Summer Heat Transfer Conference (Las Vegas, NV), 2003.
- H.B. Xiong, L.L. Zheng, J. Margolies, and S. Sampath, "Numerical Simulation of Radio Frequency Induction Plasma Spray Processing," International Mechanical Engineering Congress and Exposition (Anaheim, CA), 2004.
- H.B. Xiong, L.L. Zheng, S. Sampath, R.L. Williamson, and J.R. Fincke, "Three-Dimensional Simulation of Plasma Spray: Effects of Carrier Gas Flow and Particle Injection on Plasma Jet and Entrained Particle Behavior," *Int. J. Heat Mass Transfer,* (submitted).

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