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Project Title: A Transport Phenomena Based Approach to Probe Evolution of Weld Macro and Microstructures and A Smart Bi-directional Model of Fusion Welding

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Summary

In recent years, applications of numerical heat transfer and fluid flow models of fusion welding have resulted in improved understanding of both the welding processes and welded materials. They have been used to accurately calculate thermal cycles and fusion zone geometry in many cases. Here we report the following three major advancements from this project. First, we show how microstructures, grain size distribution and topology of welds of several important engineering alloys can be computed starting from better understanding of the fusion welding process through numerical heat transfer and fluid flow calculations. Second, we provide a conclusive proof that the reliability of numerical heat transfer and fluid flow calculations can be significantly improved by optimizing several uncertain model parameters. Third, we demonstrate how the numerical heat transfer and fluid flow models can be combined with a suitable global optimization program such as a genetic algorithm for the tailoring of weld attributes such as attaining a specified weld geometry or a weld thermal cycle.

The results of the project have been published in many papers and a listing of these are included together with a list of the graduate thesis that resulted from this project. The work supported by the DOE award has resulted in several important national and international awards. A listing of these awards and the status of the graduate students are also presented in this report.

Introduction

Although welding is a critical technology for the civilian infrastructure and national defense of the United States, the construction of structurally sound and reliable welds is still done largely by trial and error aided by experience. Since there are a large number of process variables in welding, the desired weld attributes such as the weld geometry and structure are difficult to produce. Furthermore the empirical approach does not always produce optimum welds and inappropriate choice of variables can lead to poor welds.

In many simple alloy systems, the computed thermal cycles have been used to quantitatively understand weld microstructure and inclusion structure. However, there are two major problems in the previous research. Often the thermal cycles necessary for the calculation of structures have been obtained from the cooling rates computed from the heat conduction equations. Previous work has shown that these calculations are inaccurate because they ignore the dominant mechanism of heat transfer, i.e., convective eat transport. Second the traditional weld microstructural studies using post weld characterization does not provide any pathways of the evolution of microstructures, since microstructures change during heating and cooling during welding. Through development of advanced numerical models to obtain accurate cooling rates and in-situ, real time studies of phase transformation using X-ray (synchrotron) diffraction through collaborative research with Lawrence Livermore National Laboratory (Dr. J. W. Elmer and Dr. T. A. Palmer), we have shown that microstructural evolution of welds in both carbon steel and stainless steels can be understood at a level that has never been achieved before.

Systematic tailoring of weld attributes based on scientific principles still remains an important milestone in changing welding from almost an empirical art to a mainstream science-based technology. The ability to determine multiple welding variable sets to achieve desired weld attributes, based on scientific principles, is an important step to achieve this goal. The existing transport phenomena based models of welding can only predict weld characteristics for a given set of input welding variables. What is needed, and not currently available, is a capability to systematically determine multiple paths to tailor weld geometry and assess robustness of each individual solution to achieve safe, defect free welds. Therefore, these heat transfer and fluid flow based models are restructured to predict the welding conditions to achieve welds with desired attributes.

Three main requirements are desirable in a model for systematic tailoring of a weld attributes. First, the procedure should embody an adequate phenomenological description of the complex physical processes in welding. Although the heat transfer and fluid flow models use time-tested equations of conservation of mass, momentum and energy, the predictions of temperature fields and thermal cycles do not always agree with experimental results because the models require many input variables all of which cannot be prescribed with certainty. For example, the reported values of arc efficiency vary significantly for minor differences in the surface characteristics of work pieces that are difficult to characterize for every welding process. Second, the models are designed to calculate the temperature and velocity fields for a given set of welding variables. However, very often what is needed is to determine the welding variables required to achieve a given weld attribute such as the weld geometry, cooling rate and the microstructure. The current generation of unidirectional heat transfer and fluid flow models are designed to calculate temperature and velocity fields from welding conditions and are incapable of determining welding conditions. Finally, the welding system is highly complex and involves non-linear interaction of several welding variables. As a result, a particular weld attribute such as the geometry can be obtained via multiple paths, i.e., through the use of various sets of welding variables. The current generation of numerical heat transfer and fluid flow models cannot determine alternative pathways to achieve a target weld attribute.

In this project, a new structure of the phenomenological models is developed by combining numerical heat transfer and fluid flow models with a suitable optimization procedure in the form of a genetic algorithm. The combined model has new capabilities for bi-directional simulation where either the traditional input or the output variables can be specified. The new formulation also allows determination of multiple solutions to attain a specified weld attribute. Genetic algorithms (GA) can systematically search for multiple combinations of welding variable sets that comply with the phenomenological laws of welding physics and obtain a population of solutions following certain rules of evolution. This research represents the very first effort to adapt transport phenomena based models along with genetic algorithm based optimization model to achieve welds with desired attributes.

Technical Progress

The phase transformations during fusion welding of a low-carbon steel, a stainless steel and Ti-6Al-4V alloy were investigated by a combination of experiments and modeling. The experiments involved the real-time phase mapping using the x-ray diffraction technique at Lawrence Livermore National Lab. Numerical heat transfer and fluid flow calculations were used to obtain the weld temperature distribution, heating and cooling rates under both linear and transient spot welding conditions. The computed FZ geometries using the thermo-fluid model were compared with the experimental results. A kinetic model was developed to describe the kinetics of phase transformations controlled by the nucleation and growth mechanism. The necessary kinetic parameters were computed from the x-ray diffraction data, allowing the rates of phase transformations to be predicted under various heating conditions. In particular, the kinetic parameters were determined for the α-ferrite to γ-austenite transformation in the 1005 low-carbon and 1045 medium carbon steels, and the α-Ti to β-Ti transformation in the Ti-6Al-4V alloy.

Kinetics of the γ-austenite to δ-ferrite transformation during welding of 2205 DSS was studied experimentally by the SRXRD technique and simulated using a combination of thermo-fluid and diffusion models. A numerical diffusion model employing a moving grid system to trace the moving interface was developed to calculate the kinetics of $\gamma \rightarrow \delta$ transformation during heating of the 2205 DSS. The predicted transformation kinetics agree reasonable well with those measured using the SRXRD technique at various monitoring locations in the weldment. The calculated fraction converted curve exhibits an S-shaped profile as a result of the non-isothermal heating. The TTT and CHT diagrams were calculated for the 2205 DSS using the numerical diffusion model, providing a graphical means to predict the kinetics of the $\gamma \rightarrow \delta$ transformation. Both TTT and CHT diagrams show that the transformation rate increases with temperature. A preliminary study of the effect of non-uniform starting microstructure on the transformation rate was carried out considering a system with two γ grains and two δ grains. It is found that the overall transformation rate is fastest when the starting structure is uniform. The non-uniform starting structure slows down the transformation rate, particularly towards the end of the transformation, because the small γ grains dissolve at the initial stage of the transformation, thereby reducing the δ/γ interface area. The overall reaction rate is then controlled by the dissolution of large γ grains. The variation of γ grain thickness has a more profound effect on retarding the transformation kinetics than that of δ grain thickness.

Grain size and topological class distributions in the heat-affected zone (HAZ) of gas tungsten arc welded Ti–6Al–4V alloy were measured for various heat inputs. The evolution of grain structure and topological class distributions were also calculated using a three-dimensional Monte Carlo model utilizing thermal cycles computed from a well tested numerical heat transfer and fluid flow model. Both the experimental data and the calculated results showed that the average prior-β grain size near the fusion plane was about four to twelve times larger than the average grain size in the base plate, depending on the heat input. At locations equidistant from the fusion plane, the grains were larger in the mid-section vertical symmetry plane as compared to those at the top surface due to local variations of the thermal cycles. The normalized grain size distributions were unaffected by the local differences in the thermal cycles. It is demonstrated that the presence of a spatial gradient of temperature in the HAZ significantly impeded grain growth due to thermal pinning effect. Furthermore, the steep temperature gradients near the fusion plane did not introduce any significant texture in the grains. Both the experimental data and the calculated results indicated that the grains in the HAZ of the Ti–6Al–4V alloy were significantly smaller than the grains in the commercially pure titanium for identical welding conditions.

Six neural networks have been developed for GTA welding of stainless steel. Each of these neural networks takes 17 input variables, which include welding process parameters and important material properties, and provides one output variable. The output variables include depth, width and length of the weld pool, peak temperature, cooling time from 800°C to 500°C and maximum liquid velocity in the weld pool. The networks were trained using a hybrid optimization scheme including the gradient descent method and a genetic algorithm. The hybrid approach gave lower errors than only the gradient descent method on both training and testing datasets, and the results did not depend on the initial choice of weights. The training and testing datasets contained results from the reliable numerical transport phenomena based model for GTA welding. The accurate prediction of these results by the neural networks ensured that the output of these networks complies with the phenomenological laws of welding physics.

Several uncertain parameters affect the reliability of heat transfer and fluid flow calculations welding because their values cannot be prescribed from fundamental principles.

These parameters include absorptivity of the energy, effective thermal conductivity and effective viscosity of liquid metal in the weld pool. Values of these parameters are usually adjusted by trial and error so that the computed results agree with the corresponding experimental values. We have shown that by integrating multivariable constrained optimisation with convective heat transfer and fluid flow calculations, the values of the uncertain parameters can be obtained from a limited volume of experimental data. The numerical heat transfer and fluid flow model embodying the optimized values of the uncertain parameters could accurately compute values of weld dimensions for new welding conditions. Reliability of heat transfer and fluid flow calculations can be significantly enhanced by determining the values of uncertain parameters from a limited volume of experimental data using a multivariable optimization technique with a numerical heat transfer and fluid flow model.

A bidirectional model of gas tungsten arc (GTA) welding was developed by coupling a neural network model with a real number based genetic algorithm to calculate the welding conditions needed to obtain a target weld geometry. Unlike conventional neural network models that are trained with experimental data, which predict weld geometry for a particular set of welding conditions, the proposed model could estimate the welding conditions necessary for obtaining a target weld geometry within the framework of phenomenological laws.

The model was used to determine multiple sets of welding variables, i.e., combinations of arc current, voltage and welding speed to obtain a specified weld geometry. It was found that a specific weld geometry was attainable via multiple pathways involving various sets of welding variables. Furthermore, these sets of welding variables involved significantly different values of current, voltage and welding speed. The use of a neural network model in place of numerical transport phenomena based model reduced the computation time and provided the solution within one minute. The high speed makes the neural network based model appropriate in various applications where rapid calculations are desired. Good agreement between the model predictions and the experimental data of weld pool penetration and width for various welding conditions shows that this approach is promising.

Apart from the bead-on-plate welds, the approach was also tested with fillet welds. The main computational engine used in this work is a neural network model which is trained and validated using the results of well-tested heat transfer and fluid flow model. The neural network model includes all the welding variables and material properties as input and provides weld dimensions, peak temperatures, maximum velocities and the cooling rates between 800 °C to 500 °C. This network has 22 input parameters which are connected to output layer through a hidden layer of 19 nodes. A hyperbolic tangent function (which is a symmetric *sigmoid* function) was used as the activation function to include non-linear behavior of different variables. A back-propagation algorithm was used to update the synaptic weights of the neural network. A large database of outputs for different welding conditions was generated based on design of experiments (DOE) to capture the correlations between the welding variables and the weld attributes. Separate feed forward neural networks were developed, one each for predicting penetration, leg-length and throat of GMA fillet weld in spray mode to achieve high accuracies in the calculation of penetration, leg-length and throat. The weights in the neural network models were calculated using a hybrid optimization scheme involving the conjugate gradient (CG) method and a genetic algorithm (GA). The network was trained using only the training data. The validation and testing data were randomly generated independent of the training data. The performance of the network was tested using the validation and testing datasets. The testing data was used to check the overall performance of the network. The hybrid optimization scheme helped in finding optimal weights through a global search as evidenced by good agreement between all the outputs from the neural networks and the corresponding results from the heat and fluid flow model.

The effectiveness of the model was tested by finding different sets of welding variables which could provide a specified weld geometry. The computational task involved three steps. First, a target weld geometry was selected by specifying one set of values of penetration, throat and leg-length. Second, the model was run to obtain multiple combinations of welding variable sets each of which could produce the target weld geometry. Third, and final, the results obtained from the model were adequately verified by comparing experimental results with the computed results.

Significance of the Work

With the advancement of computational hardware and software, many research projects that could not be undertaken just a few years ago can now be tried. It is demonstrated here that when numerical heat transfer and fluid flow models are combined with real time experiments, details of microstructure evolution can be studied with clarity and certainty that have not been possible before. The ability of the modern numerical models to correctly predict multiple welding variable sets that can lead to the target weld dimensions proves that by combing the principles of evolutionary biology with welding physics, a useful phenomenological framework can be created to systematically tailor a weld attribute via multiple paths. Although the work reported here focuses on tailoring of weld geometry, these results provide hope that by using the proposed approach, welding engineers will be able to tailor the structure and properties of weldments in the future.

PUBLICATIONS

1. J. W. Elmer, T. A. Palmer, W. Zhang and T. DebRoy, Time Resolved X-Ray Diffraction Observations of Phase Transformations in Transient Arc Welds, Science and Technology of Welding and Joining, 2008, vol. 13(3), pp. 265-277.
2. R. Rai, J. W. Elmer, T. A. Palmer and T. DebRoy, Heat Transfer and Fluid Flow during Keyhole Mode Laser Welding of Tantalum, Ti-6Al-4V, Stainless Steel and Vanadium, Journal of Physics D, 2007, vol. 40, pp. 5753-5766.
3. R. Rai, G.G. Roy, T. DebRoy, A Computationally Efficient Model of Convective Heat Transfer and Solidification Characteristics during Keyhole Mode Laser Welding, Journal of Applied Physics, 2007, vol. 101, article #054909.
4. A. Kumar and T. DebRoy, Tailoring Fillet Weld Geometry using a Genetic Algorithm and a Neural Network Trained with Convective Heat Transfer Calculations, Welding Journal, 2007, vol. 86(1), pp. 26s-33s.
5. S. Mishra and T. DebRoy, Tailoring Gas Tungsten Arc Weld Geometry using a Genetic Algorithm and a Neural Network Trained with Convective Heat Flow Calculations, Materials Science and Engineering A, 2007, vol. 454–455, pp. 477–486.
6. R. Nandan, S. Mishra and T. DebRoy, Tailoring Fusion and Friction Stir Welds Using a Transport Phenomena Based Reliable and Efficient Model and a Genetic Algorithm, Mathematical Modeling of Weld Phenomena 8, edited by H. Cerjak, H.K.D.H. Bhadeshia and E. Kozeschnik, Verlag der Technischen Universitat Graz, Austria, 2007, pp. 485-510.
7. G. G. Roy, J. W. Elmer and T. DebRoy, Mathematical Modeling of Heat Transfer, Fluid Flow and Solidification during Linear Welding with a Pulsed Laser Beam, Journal of Applied Physics, 2006, vol. 100(3), article #034903.
8. S. Mishra and T. DebRoy, Non-Isothermal Grain Growth in Metals and Alloys, Materials Science and Technology, 2006, vol. 22 (3), pp. 253-278.
9. S. Mishra and T. DebRoy, A Genetic Algorithm and Gradient Descent based Neural Network with the Predictive Power of a Heat and Fluid Flow Model for Welding, Welding Journal, 2006, vol. 85(11), pp.231s-242s.
10. X. He, J. T. Norris, P. W. Fuerschbach, and T. DebRoy, Liquid Metal Expulsion during Laser Spot Welding of 304 Stainless Steel, Journal of Physics D: Applied Physics, 2006, vol. 39 (3), pp. 525-534.
11. R. Rai and T. DebRoy, Tailoring Weld Geometry during Keyhole Mode Laser Welding using a Genetic Algorithm and a Heat Transfer Model, Journal of Physics, D: Applied Physics, 2006, vol. 39(6), pp. 1257-1266.

12. A. De and T. DebRoy, Improving Reliability of Heat and Fluid Flow Calculations during Conduction Model Laser Spot Welding by Multi-variable Optimization, Science and Technology of Welding and Joining, 2006, vol. 11(2), pp.143-153.

13. A. Kumar and T. DebRoy, Toward a Unified Model to Prevent Humping Defects in Gas Tungsten Arc Welding, Welding Journal, 2006, vol. 85(12), pp. 292s-304s.

14. S. Mishra, T. DebRoy and S. Chakraborty, A Transport Phenomena Based Model to Prevent Liquation Cracking in Aluminum Alloy Welds, Trends in Welding Research: Proceedings of the 7th International Conference, Pine Mountain, GA, Edited by S. A. David, T. DebRoy, J. Lippold, H. Smartt, and J. Vitek, ASM International, Materials Park, Ohio, 2006, pp. 35-40.

15. A. Kumar and T. DebRoy, Reliable Modeling of Heat and Fluid Flow in Gas-Metal-Arc Fillet Welds through Optimization of Uncertain Variables, Trends in Welding Research: Proceedings of the 7th International Conference, Pine Mountain, GA, Edited by S. A. David, T. DebRoy, J. Lippold, H. Smartt, and J. Vitek, ASM International, Materials Park, Ohio, 2006, pp. 85-90.

16. A. Kumar and T. DebRoy, Transport Phenomena and Genetic Algorithm based Window of Welding Variables to Achieve a Target Gas Metal Arc Fillet Weld Geometry, Trends in Welding Research: Proceedings of the 7th International Conference, Pine Mountain, GA, Edited by S. A. David, T. DebRoy, J. Lippold, H. Smartt, and J. Vitek, ASM International, Materials Park, Ohio, 2006, pp. 91-96.

17. X. He, J. T. Norris, P. W. Fuerschbach and T. DebRoy, Alloying Element Vaporization and Liquid Metal Expulsion during Laser Microjoining of Stainless Steel with Short Pulse, Trends in Welding Research: Proceedings of the 7th International Conference, Pine Mountain, GA, Edited by S. A. David, T. DebRoy, J. Lippold, H. Smartt, and J. Vitek, ASM International, Materials Park, Ohio, 2006, pp. 109-114.

18. W. Zhang, T. DebRoy, T. A. Palmer and J. W. Elmer, Ferrite Formation in a Duplex Stainless Steel during Controlled Heating: X-Ray Diffraction and Modeling Using Para-Equilibrium Diffusion Kinetics, Trends in Welding Research: Proceedings of the 7th International Conference, Pine Mountain, GA, Edited by S. A. David, T. DebRoy, J. Lippold, H. Smartt, and J. Vitek, ASM International, Materials Park, Ohio, 2006, pp. 939-944.

19. S. Mishra, A. Kumar, T. DebRoy and J. W. Elmer, Genetic Algorithm Based Optimization of Johnson Mehl Avarami Equation Parameters for Ferrite to Austenite Transformation in Steel Welds, Trends in Welding Research: Proceedings of the 7th International Conference, Pine Mountain, GA, Edited by S. A. David, T. DebRoy, J. Lippold, H. Smartt, and J. Vitek, ASM International, Materials Park, Ohio, 2006, pp. 1001-1006.

20. A. Kumar, W. Zhang and T. DebRoy, Improving Reliability of Modeling Heat and Fluid Flow in Complex Gas-Metal-Arc Fillet Welding – Part I: An Engineering Physics Model, Journal of Physics D, 2005, vol. 38, pp. 119-126.

21. A. Kumar and T. DebRoy, Improving Reliability of Modeling Heat and Fluid Flow in Complex Gas-Metal-Arc Fillet Welding – Part II: Application to Welding of Mild Steel, Journal of Physics D, 2005, vol. 38, pp. 127-134.

22. A. Kumar and T. DebRoy, Tailoring Complex Weld Geometry through Reliable Heat Transfer and Fluid Flow Calculations and a Genetic Algorithm, Metallurgical and Materials Transactions A, 2005, vol. 36A, pp. 2725-2735.

23. X. He, J. Elmer and T. DebRoy, Heat Transfer and Fluid Flow in Laser Microwelding, Journal of Applied Physics, 2005, vol. 97, article# 84909.

24. S. Mishra, S. Chakraborty and T. DebRoy, Probing Liquation Cracking and Solidification through Modeling of Momentum, Heat and Solute Transport during Welding of Aluminum Alloys, Journal of Applied Physics, 2005, vol. 97, article# 94912.

25. A. Kumar, S. Mishra, J. W. Elmer and T. DebRoy, Optimization of Johnson Mehl Avarami Equation Parameters for α-Ferrite to γ-Austenite Transformation in Steel Welds using a Genetic Algorithm, Metal. Mater. Trans. A, 2005, vol. 36A, pp. 15-22.

26. A. De and T. DebRoy, Reliable Calculations of Heat and Fluid Flow during Conduction Mode Laser Welding through Optimization of Uncertain Parameters, Welding Journal, 2005, vol. 84(7) , pp. 101s to 112s.

27. S. Mishra and T. DebRoy, A Computational Procedure for Finding Multiple Solutions of Convective Heat Transfer Equation, Journal of Physics, D, 2005, vol. 38, pp. 2977-2985.

28. W. Zhang, T. DebRoy, and J. W. Elmer, Integrated Modeling of Thermal Cycles, Austenite Formation, Grain Growth and Decomposition in the Heat Affected Zone of Carbon Steel, Science and Technology of Welding and Joining, 2005, 10(5), pp. 574-582.

29. W. Zhang, T. DebRoy, T. A. Palmer and J. W. Elmer, Modeling of Ferrite Formation in a Duplex Stainless Steel Weld Considering Non-uniform Starting Microstructure, Acta Materialia, 2005, vol. 53(16) pp. 4441-4453.

30. S. Mishra and T. DebRoy, A Heat Transfer and Fluid Flow Based Model to Obtain a Specific Weld Geometry Through Multiple Paths, Journal of Applied Physics, 2005, vol. 98, 044902.

31. W. Zhang, C. L. Kim and T. DebRoy, Heat and Fluid Flow in Complex Joints during Gas-Metal Arc Welding, Part I: Numerical Model of Fillet Welding, Journal of Applied Physics, 2004, vol. 95, pp. 5210-5219.

32. W. Zhang, C. L. Kim and T. DebRoy, Heat and Fluid Flow in Complex Joints during Gas-Metal Arc Welding, Part II: Application to Fillet Welding of Mild Steel, Journal of Applied Physics, 2004, vol. 95, pp. 5220-5229.

33. A. De and T. DebRoy, A Smart Model to Estimate Effective Thermal Conductivity and Viscosity in Weld Pool, Journal of Applied Physics, 2004, vol. 95(9), pp. 5230-5239.

34. X. He, T. DebRoy and P. Fuerschbach, Composition Change of Stainless Steel during Micro-joining with Short Laser Pulse, Journal of Applied Physics, 2004, vol. 96(8), pp. 4547-4555.

35. A. De and T. DebRoy, Probing Unknown Welding Parameters from Convective Heat Transfer Calculation and Multivariable Optimization, Journal of Physics, D: Applied Physics, 2004, vol. 37, pp. 140-150.

36. S. Mishra and T. DebRoy, Grain Topology in Ti-6Al-4V Welds – Monte Carlo Simulation and Experiments, Journal of Physics D: Applied Physics, 2004, vol. 37, pp. 2191-2196.

37. S. Mishra and T. DebRoy, Measurements and Monte Carlo Simulation of Grain Growth in the Heat-Affected Zone of Ti-6Al-4V Welds, Acta Materialia, 2004, vol. 52(5), pp. 1183-1192.

38. C.-H. Kim, W. Zhang and T. DebRoy, Modeling of Temperature Field and Solidified Surface Profile during Gas Metal Arc Fillet Welding, Journal of Applied Physics, 2003, vol. 94(4), pp. 2667-2679.

39. A. Kumar and T. DebRoy, Calculation of Three-Dimensional Electromagnetic Force Field during Arc Welding, Journal of Applied Physics, 2003, vol. 94(2), pp. 1267-1277.

40. H. Zhao and T. DebRoy, Macro-porosity Free Aluminum Alloy Weldments through Numerical Simulation of Keyhole Mode Laser Welding, Journal of Applied Physics, 2003, vol. 93(12), pp. 10089-10096.

41. S. A. David, R. Trivedi, M. E. Eshelman, J. M. Vitek, S. S. Babu, T. Hong and T. DebRoy, Observation of Weld Pool Solidification using Transparent Metal-Analog Systems, Journal of Applied Physics, 2003, vol. 93(8), pp. 4885-4895.

42. W. Zhang, G. G. Roy, J. Elmer and T. DebRoy, Modeling of Heat Transfer and Fluid Flow During Gas Tungsten Arc Spot Welding of Low Carbon Steel, Journal of Applied Physics, 2003, vol. 93(5), pp. 3022-3033.

43. X. He, P. Fuerschbach and T. DebRoy, Alloying Element Vaporization during Laser Spot Welding of Stainless Steel, Journal of Physics D: Applied Physics, 2003, vol. 36(23), pp. 3079-3088.

44. X. He, P. W. Fuerschbach and T. DebRoy, Heat Transfer and Fluid Flow during Laser Spot Welding of 304 Stainless Steel, Journal of Physics, D: Applied Physics, 2003, vol. 36, pp. 1388-1398.

45. J. W. Elmer, T. A. Palmer, W. Zhang, B. Wood, and T. DebRoy, Kinetic Modeling of Phase Transformations Occurring in the HAZ of C-Mn Steel Welds Based on Direct Observations, Acta Materialia, 2003, vol. 51(12), pp. 3333-3349.

46. T. Hong and T. DebRoy, Non-isothermal Growth and Dissolution of Inclusions in Liquid Steels, Metallurgical and Materials Transactions B, 2003, vol. 34B, pp. 267-269.

47. T. DebRoy, Organized Research and Development in Welding – Needs and Promises, Australasian Journal of Welding, 2003, vol. 40(2), p.2.

48. T. DebRoy, Computational Modeling: A Path to Expand the Knowledge Base in Fusion Welding, Indian Welding Journal, 2003, vol. 36 (3), pp. 59-66.

49. A. Kumar and T. DebRoy, Numerical Simulation of Electromagnetically Driven Flow in the Weld Pool during Arc Welding, 2003 ASME International Mechanical Engineering Congress and Exposition (IMECE2003-43698), Washington, D.C., November 16-21, 2003. Proceedings of the ASME Fluids Engineering Division – 2003, Editors: Asif H. Arastu, George Papadopoulos and Dennis Siginer, Book Number I00685, FED-Vol. 259, p. 833

50. H. Zhao and T. DebRoy, Computer Modeling of Keyhole Mode Laser Welding To Avoid Macro-porosity, Trends in Welding Research, S. A. David, T. DebRoy, J. C. Lippold, H. Smartt, and J. M. Vitek, (Editors), ASM International, Materials Park, Ohio, 2003, pp. 118-123.

51. W. Zhang, J. W. Elmer and T. DebRoy, Modeling of Ferrite to Austenite Transformation and Real Time Mapping of Phases during GTA Welding of 1005 Steel, Trends in Welding Research, S. A. David, T. DebRoy, J. C. Lippold, H. Smartt, and J. M. Vitek, (Editors), ASM International, Materials Park, Ohio, 2003, pp. 180-185.

52. S. Mishra and T. DebRoy, Grain Growth in the Heat-Affected Zone of Ti-6Al-4V Welds: Measurements and Three Dimensional Monte Carlo Simulation, Trends in Welding Research, S. A. David, T. DebRoy, J. C. Lippold, H. Smartt, and J. M. Vitek, (Editors), ASM International, Materials Park, Ohio, 2003, pp. 197-202.

53. W. Zhang, J. W. Elmer, and T. DebRoy, Modeling and Real Time Mapping of Phases during GTA Welding of 1005 Steel, Materials Science and Engineering A, 2002, vol. 333, no. 1-2, pp. 320-335.

54. W. Zhang, J.W. Elmer and T. DebRoy, Rate of Ferrite to Austenite Transformation during Heating of 1005 Steel, Scripta Materialea, 2002, vol. 46, No. 10, pp. 753-757.

55. W. Zhang and T. DebRoy, Modeling of Solidified Free Surface Profile during GMA Welding, in "Mathematical Modeling and Information Technology in Welding and Related Processes", Conference Proceedings Edited by V. I. Makhnenko, Publisher: Patton Electric Welding Institute of Ukraine, Kiev, Ukraine, 2002, pp. 24-30.

56. T. DebRoy, H. Zhao, W. Zhang and G.G. Roy, Weld Pool Heat and Fluid Flow in Probing Weldment Characteristics, Mathematical Modeling of Weld Phenomena 6, H. Cerjak, editor, Institute of Materials, 2002, pp. 21-42.

57. T. Hong and T. DebRoy, Effects of Time, Temperature and Steel Composition on the Growth and

Dissolution of Inclusions in Liquid Steels, Ironmaking and Steelmaking, 2001, vol. 28, No. 6, pp. 450-454.

58. S. Sista and T. DebRoy, Three Dimensional Monte Carlo Simulation of Grain Growth in Zone Refined Iron, Metallurgical and Materials Transactions B, 2001, vol. 32B, pp. 1195-1201.

59. H. Zhao and T. DebRoy, Weld Metal Composition Change during Conduction Mode Laser Welding of 5182 Aluminum Alloy, Metallurgical and Materials Transactions B, 2001, vol. 32B, pp. 163-172.

60. A. Robert and T. DebRoy, Geometry of Laser Spot Welds from Dimensionless Numbers, Metallurgical and Materials Transactions, B, 2001, vol. 32B, pp. 941-947.

61. H. Zhao and T. DebRoy, Pore Formation during Laser Welding of Die-cast Magnesium Alloy AM60B - Mechanism and Remedy, Welding Journal, 2001, vol. 80, No. 8, pp. 204s-210s.

62. T. Hong and T. DebRoy, Time-Temperature-Transformation Diagrams for the Growth and Dissolution of Inclusions in Liquid Steels, Scripta Materialea, 2001, vol. 35, pp. 847-852.

63. T. DebRoy and S. Kou, Heat Flow in Welding, Chapter 3, Welding Handbook, vol. 1, 9th Edition, American Welding Society, 2001, pp. 87-113.

64. T. DebRoy, Mathematical Modeling of Fluid Flow and Heat Transfer in Fusion Welding, Mathematical Modeling of Weld Phenomena 5, Edited by H. Cerjak and H.K.D.H. Bhadeshia, The Institute of Materials, London, 2001, pp. 1-31.

AWARDS AND HONORS

- **Charles H. Jennings Memorial Award,** American Welding Society, "*for the most valuable paper published by a college student or faculty in Welding Journal during the previous calendar year*," 2007, shared with A. Kumar.

- **Kennametal Fellowship** to Mr. R. Rai for scholastic accomplishments during graduate studies. His thesis research is on "*Numerical Simulation of Heat Transfer and Fluid Flow in Laser and Electron Beam Welding*." (2007).

- **Henri Granjon Prize** of International Institute of Welding, Villepinte, France to Dr. W. Zhang for best doctoral thesis in welding in any year (2006). His thesis was on "Probing Heat Transfer, Fluid Flow and Microstructural Evolution during Fusion Welding of Alloys."

- **Charles H. Jennings Memorial Award,** American Welding Society, "*for the most valuable paper published by a college student or faculty in Welding Journal during the previous calendar year*," 2006, shared with A. De.

- **Yoshiaki Arata Award,** International Institute of Welding (IIW), Villepinte, France *"given to a person who has realized outstanding achievements in welding science and technology, and its allied areas, and which have been recognized as a great contribution to the progress of welding engineering and related fields,"* 2006.

- **William Spraragen Memorial Award**, American Welding Society (AWS), "*for the best research paper printed in the Welding Journal during the twelve month period ending with the December issue*," 2005. (shared with W. Zhang, T. A. Palmer and J. Elmer)

- **Second Prize, Materials Science and Engineering Departmental Poster Contest** to Mr. A. Kumar. His poster was entitled "A Bi-directional Model to Calculate Weld Geometry using a Phenomenological Model, a Neural Network and Evolutionary Principles" (2005).

- **First Prize, Materials Science and Engineering Departmental Group Poster Contest** to Mr. W. Zhang, X. He, A. Kumar, S. Mishra and Y. Fan. Their poster was entitled "Computational Materials Processing" (2004).

- **Kenneth Easterling Best Paper Award,** International Institute of Welding, Villepinte, France and Technical University of Graz, Graz, Austria, "*for the best research paper presented at the 7th International Seminar on Mathematical Modeling of Welding," Graz, Austria*, 2003 (shared with A. Kumar, W. Zhang, and C. L. Kim)

- **Honorary Membership Award**, American Welding Society, "*this award is presented to a person of acknowledged eminence in the welding profession or who is credited with exceptional accomplishments in the industry",* 2003.

- **ASM International Visiting Lectureship Award,** ASM International, "*for lectures in India based on qualifications of the lecturer,"* 2003.

- **Best of Show Award** in a poster contest in the Department of Materials Science and Engineering, Penn State to Mr. W. Zhang. His poster was entitled "*Modeling of Macro and Microstructure during Welding*" (2001).

GRADUATE THESIS AND STATUS OF STUDENTS

1. B. Ribic, passed Ph. D. candidacy exam, likely to complete Ph.D. in Spring 2010.
2. R. Rai, Modeling Heat Transfer and Fluid Flow in Keyhole Mode Laser Welding, Ph.D. in December 2008, currently Senior Research and Development Engineer with Hawthorne and York International, Phoenix, AZ.
3. A. Kumar, Tailoring Weld Attributes using a Genetic Algorithm and a Neural Network Trained with Convective Heat Transfer Calculations, Ph. D., June 2006, currently with Exxon-Mobil, Houston, TX.
4. S. Mishra, Improving Reliability of Convective Mass Transfer Calculations in the Arc Welding of Steels using a Genetic Algorithm and a Neural Network, Ph. D., June 2006, currently Assistant Professor, IIT Bombay, India.
5. X. He, Momentum, Heat Transfer and Fluid Flow and Mass Transfer in Laser Welding of Stainless Steel with Small Scale, Ph.D., December 2005, currently with University of Michigan.
6. W. Zhang, Probing Heat Transfer, Fluid Flow and Microstructure Evolution During Fusion Welding of Alloys, Ph.D., August 2004, currently Research and Development Staff Member, Materials Joining Group, Oak Ridge National Laboratory.

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