Final Report on DOE Grant DE-FG02-84ER45158

Role of Transport Phenomena in the Evolution of Geometry, Composition and Structure

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Abstract

Fusion welding is used extensively in industries that support the nation's energy supply, defense, infrastructure, and standard of living. Safety and reliability of the welded joints are affected by their geometry, composition and structure. This report provides an account of the significant advances made in quantitative understanding of the geometry, composition and various aspects of the weldment structure with financial support from DOE/BES. In particular, this report provides an account of the research conducted under the grant DE-FG02-84ER45158 in this important area and lists all the publications that document the details of the technical accomplishments that resulted from the work. Investigations of heat transfer, fluid flow and alloying element vaporization during laser welding resulted in a new technique for the determination of the peak temperature in the weld pool and provided a new method to estimate weld metal composition. Studies on the interfacial phenomena in fusion welding resulted in quantitative understanding of the interrelationship between the weld metal composition and geometry and provided new knowledge as to when the surface active elements would affect the weldment geometry and when these elements would have no effect on the geometry. Partitioning of oxygen nitrogen and hydrogen between the welding environment and the weld metal was affected by the extent of the dissociation of diatomic gaseous species which depended on the nature of the plasma formed during welding. The interfacial tension of the liquid metal was also affected by the plasma and the properties of the plasma affected the concentrations of oxygen, nitrogen and hydrogen in the weld metal. Apart from the understanding of the evolution of composition and geometry of the weldments, application of transport phenomena provided useful information about various features of the weldment structure. Quantitative understanding of microstructure of the fusion zone and heat affected zone and grain structure in both steels and titanium alloys could be achieved starting with numerical heat transfer and fluid flow calculations. In addition, the evolution of inclusion composition and structure in steels during welding could also be understood from fundamental principles.

The positions of the students supported by the grant are indicated since an important component of the work was the education of many outstanding students who now occupy leadership positions in major organizations in the US. The research sponsored by the Basic Energy Sciences has been recognized by many major scholastic awards. These are listed because they testify to the quality of the curiosity and the commitment of the students that were

supported by the grant. Our collaborations with Oak Ridge National Laboratory, Lawrence Livermore National Laboratory and Sandia National Laboratory are indicated because many outstanding scientists from these laboratories shared our goals in advancing quantitative understanding of fusion welding processes and the geometry, composition and structure of welded materials.

Research objectives

The welding related expenditure in the U.S. in the year 2000 was approximately $34 billion, equivalent to about $325 per household. The large economic impact of welding originates from its extensive use in industries that support the nation's energy supply, defense, infrastructure, and standard of living. Fusion welding processes are complex because several physical processes such as heat and mass transfer, fluid flow, chemical reactions and phase transformations take place simultaneously during welding. Because of its complex nature, fusion welding has evolved mostly as an empirical technology. Since there are a large number of process variables in welding, the desired weld attributes such as the weld geometry and structure are commonly produced by empirically adjusting the welding variables. However, this approach does not always produce optimum welds and inappropriate choice of variables can lead to poor welds.

Systematic quantitative understanding of fusion welding processes and welded materials can save life and property by preventing catastrophic failures of large welded structures. Safety and reliability of the welded joints are affected by their geometry, composition and structure. The goal of the research was to quantitatively understand the evolution of geometry, composition and structure of welds starting from heat transfer, fluid flow and mass transfer calculations.

Technical accomplishments

During laser welding of stainless steels containing volatile components, the composition of the weld metal was significantly different from the composition of the base metal at low laser powers,, primarily because of the loss of manganese from the weld pool. The change in the composition was affected by the vaporization rate and the size of the weld pool, the latter being the dominant factor in most cases. The computed values of the vaporization rates of various alloying elements and the vapor composition were found to be in good agreement with the experimental results for welding with a sub-kilowatt power CO_2 laser. Although the rate of vaporization of alloying elements increased with the increase in the laser power, the composition change was most pronounced at low laser powers because of the small size of the weld pool. The rates of vaporization of the alloying elements were found to be independent of both the gas flow rate and the nature of the shielding gas. The most important factor for the alloying element loss was found to be the plasma influenced intrinsic vaporization at the weld poo1 surface.

The role of plasma was determined by physical simulation experiments. Rates of vaporization of pure metal drops and metal drops that were doped with small amounts of oxygen and sulfur were found to decrease when plasma was present. These results were consistent with the presence of a charge distribution field near the liquid metal surface when plasma was present. The presence of plasma lowered the interfacial tension of both iron and copper, which is consistent with the presence of a space charge effect. The temperature coefficient of interfacial tension, which affects weld penetration, did not change significantly when plasma was present. The intensity and the direction of the convection current and the accompanying heat transfer are influenced by the temperature coefficient of interfacial tension. A procedure was developed to calculate the temperature coefficient of interfacial tension using Gibbs and Langmuir adsorption isotherms. It was demonstrated that when the surface tension was calculated by using a model for the prediction of surface tension as a function of composition and temperature excellent agreement was achieved between the theoretically predicted and experimentally observed fusion zone geometry.

A novel technique for the determination of laser weld pool temperature was presented, i.e., the relative rates of vaporization of any two elements from the molten pool can serve as an indicator of the weld pool temperature, irrespective of the element pair selected. The weld pool temperatures were found to be in the range of 2900 – 3400 K, which was in reasonable agreement with the effective weld pool temperature obtained from the vapor composition measurements. The weld pool temperature was found to increase mildly with the increase in laser power under the conditions of the experiments. The variation in the welding speed did not influence the pool temperature significantly.

The results of numerical simulation of heat transfer and fluid flow in the weld pool strongly depend on the physical processes considered and the input data used in the model. The results indicated that absorptivity of CO_2 laser, viscosity, thermal diffusivity and the temperature coefficient of surface tension are the most crucial parameters for realistic simulation of the weld pool behavior. A model was developed for the calculation of surface tension of the Fe-Ni-Cr-S alloys as a function of bath temperature and composition. The results indicated that, in most cases, the surface tension data for the Fe-S system can be used for the calculation of heat transfer and fluid flow in the Fe-Cr-Ni-S system. A new technique was developed to measure the absorptivity of CO_2 laser, which was based upon the analysis of heat flow and required measurement of transient temperature profiles at various monitoring locations in the solid region of the samples during welding. The measured values of absorptivity were found to lie in the range of 0.1 to 0.2 for 0.7 mm thin samples of AISI 202 stainless steels with surface polished with standard 240 grit polishing paper. The extent of absorption of laser beam in various grades of stainless steels could be significantly improved by suitable surface modifications. The numerical calculations of heat transfer and fluid flow indicated the presence of strong recirculatory flows in the weld pool with maximum velocity as high as 80 cm/s. The weld pool shapes predicted by the model were found to be in good agreement with those obtained experimentally. The microstructure data for AISI 202 stainless steel weld was collected using SEM and TEM. Weld microstructure contained duplex austenite and ferrite at low welding speeds and was fully austenite at high welding speeds.

During pulsed laser welding, liquid metal is often expelled from the weld pool. Lead, titanium and stainless steel samples were irradiated by single and multiple pulses of CO_2 laser of varying power and pulse duration to investigate the conditions for liquid expulsion. It was demonstrated that by balancing surface tension and recoil forces, the conditions for the initiation of the liquid metal expulsion could be determined. The concentrations of interstitial impurities such as nitrogen, oxygen and hydrogen affect the structure and properties of the weld metal. Physical modeling and thermochemical calculations were conducted to understand the partition of interstitial impurities between the weld pool and its environment. The results showed that the enhanced solubility during welding can be attributed to the existence of excited atoms and perhaps other species in the welding environment.

A comprehensive model was developed, which integrated the calculations of heat transfer and fluid flow in the weld pool and the rates of vaporization and alloying element loss occurring during conduction mode laser welding. The model predictions of weld pool geometry, vaporization rates, and composition changes agreed well with the corresponding experimental results for laser welding of aluminum alloy 5182.

The time-temperature-transformation (TTT) diagrams of growth and dissolution of various types of inclusions show that Al_20_3, $MnOA1_2O_3$, and Ti_3O_5 are always the most stable oxide inclusions in the weld pool for the steel composition studied in the present research. However, alloy composition affects the relative stabilities of inclusions dramatically. The non-isothermal behavior of growth and dissolution of individual inclusions was predicted from their isothermal growth behavior by constructing continuous-cooling-transformation (CCT) diagrams for growth and continuous-heating-transformation (CHT) diagrams for dissolution of inclusions. A well tested numerical fluid flow and heat transfer model that considers turbulence was used to calculate the temperature and velocity fields in the weld pool.

Due to the fluid flow in the weld pool the nuclei of inclusions undergo vigorous motion. During the residence time of inclusions in the liquid bulk alloy, they experience both growth and dissolution. Particle tracking results showed that most inclusions experience complex gyrations and thermal cycles before they are trapped on the solid region in the weldment. The temperature versus time plots of the inclusions in many cases displayed several characteristic temperature peaks. However, about one-third of the particles experienced continuous cooling behavior, i.e., no temperature peak. Thermal cycles of thousands of inclusions nucleated in the weld region were tracked and their growth and dissolution was calculated to obtain the final size distribution and number density of inclusions statistically. The computed results showed that inclusion size distributions are affected by the welding parameters and alloy composition. The inclusions are coarser at low welding speeds and high welding powers. Good agreement was found between the computed and the experimentally observed inclusion size distribution. The collision and coalescence model was applied to modify the calculated number density of single kind of inclusions. With the increase of time, the number densities of smaller size inclusions became lower. The entire distribution profile became more uniform in size and the average size became higher.

The effect of turbulence on the heat transfer and fluid flow in the weld pool was studied. The rigorously calculated results from the three dimensional thermofluid model indicated that the heat transfer and fluid flow in the weld pool was significantly enhanced by turbulence in many cases, particularly when high heat input was used. The “finger penetration”, a unique geometric feature of gas metal arc (GMA) welding, was satisfactorily predicted.

In low alloy steel weldments, the weld metal microstructure is a function of both chemical composition and cooling rates. The effects of chemical composition and cooling rates on the weld metal microstructure were satisfactorily predicted in C-Mn steels and HSLA-100 steel by coupling the continuous-cooling-transformation (CCT) diagrams obtained from a well tested phase transformation model and the cooling rates calculated from the comprehensive thermal model. The mathematical modeling was combined with real-time experiments to investigate the phase transformation mechanism in the HAZ of commercially pure titanium. The mechanism of the α-Ti $\rightarrow$ β-Ti transformation during heating was identified by a comparison of the experimental results with kinetic data obtained from modeling assuming various possible mechanisms.

The grain growth phenomenon in the HAZ is complicated due to the steep temperature gradients and rapid thermal cycling in this region. The salient features of the grain growth and grain topology in the entire HAZ of commercially pure titanium welds considering the steep temperature gradients and transient thermal cycles were effectively simulated by coupling the three-dimensional (3D) Monte Carlo (MC) model with the 3D thermofluid model. The spatial distribution of grain size in the HAZ could be quantitatively predicted. Similarly the topological class distribution was also calculated.

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Collaborations

Dr. Stan A. David, Oak Ridge National Laboratory

Dr. John A. Vitek, Oak Ridge National Laboratory

Dr. John W. Elmer, Lawrence Livermore National Laboratory

Dr. Phillip W. Fuerschbach, Sandia National Laboratory

Awards and honors

- **William Spraragen Memorial Award** (T. DebRoy), American Welding Society (AWS), "*for the best research paper printed in the Welding Journal during the twelve month period ending with the December issue*," 2001. (shared with Z. Yang, J. Wong and J. Elmer)

- **The 57th Comfort A. Adams Lecture of American Welding Society** (T. DebRoy)**.** The Society describes this award as follows: "*An award is made annually by the AWS Board of Directors to an outstanding scientist or engineer whose lecture presents some new and distinctive development in the field of welding*," 2000.

- **Fellow, American Welding Society** (T. DebRoy) **"***in recognition of outstanding and distinguished contributions that have enhanced the advancement of the science, technology and application of welding***,"** 1999.

- **Warren F. Savage Memorial Award** (T. DebRoy)**,** American Welding Society, "*for innovative research resulting in a better understanding of the metallurgical principles related to welding,"* 1998. (shared with K. Mundra, S. Babu and S. A. David)

- **Charles H. Jennings Memorial Award** (T. DebRoy)**,** American Welding Society, "*for the most valuable paper published by a college student or faculty in Welding Journal during the previous calendar year,*" 1997. (shared with W. Pitscheneder, K. Mundra and R. Ebner)

- **Faculty Scholar Medal** (T. DebRoy), The Pennsylvania State University, "*for outstanding achievement in engineering"*, maximum five Faculty Scholar Awards are made per year from among approximately 4200 Penn State faculty, 1997.

- **McKay Helm Award** (T. DebRoy), American Welding Society, *"for the best technical paper on the welding of steel published in the Welding Journal in the previous calendar year,*" 1994. (shared with K. Mundra)

- **Wilson Research Award** (T. DebRoy), College of Earth and Mineral Sciences, The Pennsylvania State University, "*for outstanding contributions to the understanding of weld pool surface phenomena*," 1993.

- **Fellow, ASM International** (T. DebRoy), "*for pioneering fundamental research in welding…and for leading efforts in the mathematical modeling of welding processes*," 1993.

- **Adams Memorial Membership Award** (T. DebRoy)**,** American Welding Society, "*for outstanding teaching*," 1992.

- **Kennametal Fellowship** to Mr. W. Zhang. For scholastic accomplishments during graduate studies. His thesis research is on "*Heat Transfer, Fluid Flow and Phase Transformation Kinetics during Fusion Welding*." (2002)

- **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)

- **Geoffrey Belton Award** of American Iron & Steel Society to Dr. T. A. Palmer. For best doctoral thesis on iron and steel. His thesis was entitled "*Nitrogen in Plasmas and Steel Weld Metal*." (2001)

- **American Welding Society Fellowship** ($25,000 per year for three years)to Mr. W. Zhang. For doctoral thesis research. (2000)

- **ASM International Graduate Student Paper Contest Winner**, Mr. T. A. Palmer. His research paper was entitled "A study of nitrogen dissolution into the weld metal during arc welding". (November 1999).

- **American Council winner, Granjon International Prize Competition** to Mr. T. A. Palmer. Based on a technical paper authored by a college student. (1997-98)

- **American Welding Society Foundation Fellowship** ($25,000 per year for three years) to Mr. T. A. Palmer for research on "Partition of Nitrogen between Weld Metal and its Plasma Environment." (1995-1998)

- **Second Prize, Student Poster Contest**, 76th Annual Meeting of the American Welding Society, Cleveland, OH to Mr. T. A. Palmer. (1995)

- **McKay Helm Award** of American Welding Society to Mr. K. Mundra. For the best technical paper on the welding of steel published in the Welding Journal in the previous calendar year. (shared with T. DebRoy) (1994)

- **Dow Chemical Award** to Mr. K. Tankala. For outstanding doctoral thesis research. (1994).

- **Graduate School Fellowship of** The Pennsylvania State University to Mr. H. Venugopalan. (1993-94)

- **First Prize, Student Poster Contest,** 74th Annual Meeting of American Welding Society, Houston, TX to Mr. K. Mundra and Mr. D. Madey. (1993)

- **Second Prize, Student Poster Contest**, 74th Annual Meeting of American Welding Society, Houston, TX, to Mr. K. Mundra. (1993)

- **American Vacuum Society Award** to Mr. K. Tankala. For outstanding scholarship, (1992)

- **First Prize, Student Poster Contest**, 73rd Annual Meeting of American Welding Society, in Chicago, Ill to Mr. K. Mundra. (1993)

Student training and current positions

1. T. Hong, Modeling Growth and Dissolution of Inclusions During Fusion Welding of Steels, Ph.D. Thesis, May 2003. (currently with Caterpillar, Inc, Peoria, IL)

2. S. Mishra, Grain Growth in the Heat Affected Zone of Ti-6Al-4V Alloy Welds Measurements and Monte Carlo Simulations, M.S. Thesis, May 2003, currently pursuing Ph.D. work at Penn State..

3. Y. Fan, The Effect of Torch Angle on Fluid Flow and Heat Transfer during GTA Welding, M.S. Thesis, Spring 2003, currently pursuing Ph.D. at Columbia University.

4. H. Zhao, Quality Issues in Laser Welding of Automotive Aluminum and Magnesium Alloys, Ph. D. Thesis, December 2001. (currently Senior Scientist, Medtronic, Inc., Brooklyn Center, MN)

5. S. Sista, Computer Simulation of Grain Growth in Three Dimensions by Monte Carlo Technique, M.S. awarded: December 2000. (currently with Intel, Hillsboro, OR)

6. Z. Yang, Modeling Weldment Macro and Microstructure from Fundamentals of Transport Phenomena and Phase Transformation Theory, Ph.D. awarded: May 2000. (currently with Caterpillar, Inc, Peoria, IL)

7. T. A. Palmer, Nitrogen Plasmas and Steel Weld Metal, Ph.D. awarded: August 1999. (currently with Lawrence Livermore National Laboratory)

8. H. Guo, Laser Assisted Cleaning of Oxide Films on 409 Stainless Steel, M.S. awarded: May 1999. (currently with Hobert Brothers, Troy, OH)

9. M. Pastor, Pore Formation and Determination of Parameters for Laser Welding of Aluminum Alloys 5182 and 5754, M.S. awarded: August 1998. (currently Professor of Mechanical Engineering, Ecuador)

10. T. A. Palmer, Thesis topic: Physical Modeling of Nitrogen Partition between the Weld Metal and its Plasma Environment, M.S. awarded: May 1996. (currently with Lawrence Livermore National Laboratory)

11. D. Madey, Thesis topic: Interactions between Silver and Microwave Induced Oxygen Plasma, M.S. Awarded: May 1995.

12. K. Mundra, Thesis topic: Interfacial Phenomena in Welding: Vaporization and Gas Dissolution, Ph.D. awarded: May 1994. (currently with General Electric, Schenectady, NY)

13. S. Basu, Thesis topic: Rapid Vaporization during Pulsed Carbon Dioxide Laser Welding, M.S. Awarded: August 1992. (currently Assistant Professor of Mechanical Engineering, Temple University)

14. R. Miller, Thesis topic: Plasma Temperature, Electron Density, and Laser Beam Transmission during Laser Welding of Stainless Steels, M.S. Awarded: May 1989. (currently with Hart Metals, Tamaqua, PA)

15. M. M. Collur, Thesis topic: Alloying Element Vaporization and Emission Spectroscopy of Plasma During Laser Welding of Stainless Steels, Ph.D. awarded: December 1988. (currently with Hoffman Industries, Reading, PA)

16. P. Sahoo, Thesis topic: Interfacial Phenomena in Welding, Ph.D. awarded: August 1988. (currently with Sulzer Hickham Inc., La Porte, TX)

17. S. A. Abdulgadar*, Thesis topic: Laser Welding of 200-Series Stainless Steels Solidification Behavior and Microstructural Characteristics, Ph.D. awarded: August 1988.

18. T. Marsico, Thesis topic: Mass Transfer Studies of Laser Welded Aluminum Alloys 5083 and 7039, M.S. Awarded: May1988.

19. A. J. Paul, Thesis topic: Fluid Flow and Heat Transfer in Laser Melted Pools, Ph.D. awarded: August 1987. (currently with IBM Global Services)

20. P. A. A. Khan, Thesis topic: Mass Transfer During Laser Welding of High Manganese Stainless Steels, Ph.D. awarded: August, 1987. (currently General Manager, Pakistan Steel)

21. J. Sychterz, Thesis topic: Fluid Flow and Inclusion Removal in a Continuous Casting Tundish, M.S. Awarded: May 1984. Engineering and Planning Officer, Portsmouth Naval Shipyard, Portsmouth, NH.

Acknowledgement

The research described in this report was made possible with support from the Basic Energy Sciences Division of the US Department of Energy. We are especially grateful to have had an opportunity to work with an exceptionally knowledgeable professional, Dr. Yok Chen, who sets a very high standard of public service through his dedication to the goals of DOE/BES, his fairness, and helpfulness.