ADMINISTRATIVE INFORMATION

1. **Project Name:** Development and Implementation of Advanced Wear and Corrosion Resistant Systems Through Laser Surface Alloying and Materials Simulation

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5. **Date Project Initiated:** June 1, 2004

6. **Expected Completion Date:** May 31, 2006

PROJECT RATIONALE AND STRATEGY

7. **Project Objective:** The program involves the development of processing and material simulation techniques for identifying and creating advanced coatings through the laser surface alloying (LSA) process. This will be accomplished through theoretical analyses, augmented by laboratory experimentation, to develop and verify advanced composite coating systems and laser processing technology that may be transferable to industry.

8. **Technical Barrier(s) Being Addressed**: Technical barriers that are being addressed under this program include:

    (1) availability of precise thermodynamic data for the many material components that are of interest,
    (2) accurate depiction of microstructural data via an integrated process and materials model, and
    (3) ability to control heat input to prevent dissolution of hard particles, which is one of the most common unwanted microstructural modifications that may occur during production of composite coating systems.

9. **Project Pathway:** Accurate thermophysical properties are being acquired for the material systems of interest. This includes accumulation of specific reference thermophysical data, as well as acquiring thermophysical data bases that have been generated for computation thermodynamic calculations. The present simulation techniques rely on manual passing of thermal history to the thermodynamic and kinetic models to predict microstructural evolution. To support virtual-based development of the material and process requirements, process and materials models are being developed and integrated to allow numerical heat transfer with computational thermodynamic and kinetic models to predict the microstructural evolution in laser surface modified regions. The coupled models are also being utilized to identify processing conditions and material systems that minimize heat input while maximizing deposition, such as the use of distributed heat sources of direct diode lasers, to ensure survivability of coating having hard, second phase particles.

10. **Critical Technical Metrics:** Success of the first year of this program will be measured against four metrics. These are:

    (1) refining the simulation techniques and integration of the components into a single system capable of predicting composite coating microstructures for two broad material systems,
    (2) identifying and collecting thermodynamic data on these two material systems that is capable of depicting a wide range of processing conditions,
    (3) conducting detailed analysis sessions, with direct input of the industrial partners, using the integrated simulation system that are directed at specific coating applications, and
    (4) conducting initial tests for validation of the coatings for these specific applications.

PROJECT PLANS AND PROGRESS

11. Past Accomplishments: The heat transfer model for the laser surface alloying process was completed. The model utilizes a three-dimensional explicit finite differencing scheme, and utilizes variable grid spacing in two dimensions (the thickness and width) and a fixed spacing in the third dimension (length) to reduce computational time. It is capable of time-dependent analysis, as well as quasi-steady state calculations. The model is capable of varying substrate size, powder layer thickness, and position of clad scan. The model also incorporates two sets of properties that are used to define the porous powder and the substrate. Because of the importance in energy transfer efficiency in the heat transfer model, numerous calorimetric experiments were conducted to determine the effective absorption coefficient for a Nd:YAG laser beam irradiating and iron and nickel-based powders. A relationship, that has previously not been available, has been developed to describe bulk absorption of powders in three-dimensional spatial representation. This sub-model has been developed from

closely controlled experiments that were designed to measure powder absorption through thickness for Nd:YAG (λ=10,600 nm) and CO_2 (λ=1,064 nm) irradiation.

A survey was conducted to identify composite coating systems of interest. This was used to guide detailed materials simulations, and primarily involved the analysis of carbides in Fe-Cr matrix alloys. This particular system would be anticipated to show good corrosion resistance and significant improvements in wear resistance associated with the hard, martensitic matrix and the hard carbide particles.

Process and materials simulation was used determine specific carbide and nitride particles that have potential as composite coatings, based the on Fe-Cr matrix alloys identified above. This resulted in a matrix of experimental conditions that included laser surface alloying of a mild steel substrate with a martensitic grade of stainless steel, A431, and the addition of hard particles, TiN, TiC, and WC. The thermodynamic analysis also indicated the potential for shielding gas to influence the retained microstructure of the coating. Experiments were conducted using TiC and alloy 431 powder produced in air, argon, and nitrogen shielding gas. The experimental results indicated that the deposits produced in argon retained some TiC particles and a modest increase in hardness when compared to deposits produced using only the 431 powder. It was also found that the laser deposits of TiC and alloy 431 powder produced using active nitrogen shielding gas resulted in hardness values significantly higher than those achievable with current hardfacing powders, owing to the establishment of microstructures retaining some TiC particles, as well as fine precipitates of Ti(CN) formed during cooling.

Simulation sessions were conducted at Oak Ridge National Laboratory with selected industry representatives. This included detailed thermodynamic analysis of the REX^{TM} family of powders (Fe-Co-Mo-W-Cr-Va-C alloys) with various hard particles. Analyses were conducted on the REX materials potentially containing WC and TaC particles. Additional analyses were conducted with Stellite^{TM} 6 containing HfC and TaC, as well as nickel-based matrices with TiB_2. Results indicated potential stability of these combinations and will be experimentally validated.

12. **Future Plans:** Key milestones and deliverables for this program are shown below.

Phase I (Year 1) Milestones and Deliverables:

(1) Refinement and integration of simulation techniques that provides predictive capabilities for describing the resultant composite structures. The thermodynamic analyses have been utilized successfully, and confirmed experimentally, for several materials systems. The process model is currently under beta-testing with the industrial partners.

(2) Verification of theoretical analyses by designing advanced coating systems applicable to industry. This will include an experimental verification. Approach has been utilized to design coating of interest. These composite coatings have been verified experimentally.

Phase II (Year 2) Milestones and Deliverables:

(1) Industrial demonstration of processes and materials for three applications that utilize advanced laser-based coating technology.

(2) Confirmation of enhanced performance of the technology and industrial implementation for improving efficiency and extended life of wear and corrosion critical components. This will also include a final report specifying improvements.

Date	Milestone/Deliverable	Partner Activities
4-30-05	1-1: Refine simulation techniques	ARL Penn State and ORNL
4-30-05	1-2: Verify theoretical analysis	ARL Penn State and ORNL
4-30-06	2-1: Industry demonstration	Alvord Polk, Spirex, Praxair
4-30-06	2-2: Confirm enhanced performance	Alvord Polk, Spirex, Praxair

13. **Project Changes:** The program start has been delayed due to fulfilling program contacting requirements. This has been addressed, and the program began June 1, 2004.

14. **Commercialization Potential, Plans, and Activities:** The program team has been selected to provide efficient transitioning of the technology to commercialization. Considerations of the potential applications of advanced composite coating technologies, having the greatest impact on reducing energy and improving component life, have been integrated into the project plan at the earliest possible stage. The approach of direct industry input for identifying applications of interest, continued collaboration with industry during development, followed by industrial site demonstrations, ensures a direct path to commercialization. The participants chosen for this team provide the expertise in their respective areas to successfully accomplish technical development and commercial implementation of advanced composite coatings technologies. Potential applications for the advanced coatings have been identified by the industrial partners. Materials analyses for these applications have been completed and the program is now concentrating on identifying the process envelope for final validation and performance testing.

15. **Patents, Publications, Presentations:**

1 Martukanitz, R. P. and Babu, S. S., Development of Advanced Coatings for Laser Modifications Through Process and Materials Simulation, Proceedings of the 8th International Conference on Numerical Methods in Industrial Forming Processes, American Institute of Physics, submitted, 2004.

2. Babu, S. S., Kelly, S. M., Murugananth, M., and Martukanitz, R. P., The Use of Reactive Gas Shielding for Production of Hard Coatings by Laser Surface Alloying, Proceedings of the 23rd International Congress on Applications of Lasers & Electro-Optics, Laser Institute of America, Vol. 97, 606-612, 2004.
3. Boyer, R. and Martukanitz, R., Laser Deposition of Tool Grade Material, Industrial Laser Solutions for Manufacturing, Vol. 19 (11), 23-25, 2004.
4. Martukanitz, R. P., Melnychuk, R. M., and Copley, S. M., Dynamic Absorption of a Powder Layer, Proceedings of the 23rd International Congress on Applications of Lasers & Electro-Optics, Laser Institute of America, Vol. 97, 1404-1409, 2004.
5. Naber, A. and Martukanitz, R., A Phase-field Model for Simulation of the Laser Cladding Process Using a Discontinuous Viscosity Variable and Its Approximation by Finite Element Method, Proceedings of the 23rd International Congress on Applications of Lasers & Electro-Optics, Laser Institute of America, Vol. 97, P536-P539, 2004.
6. Martukanitz, R., Naber, A., and Melynchuck, R. Improving the Understanding of Laser Deposition Processes Through Process Simulation, Proceedings of the 7th International Conference on Trends in Welding Research, ASM International, June 2004.