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Predictive Model and Methodology for Heat Treatment Distortion Final Report CRADA No. TC-298-92

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Final Report

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Date Technical Work Began: January 1994

Date Technical Work Ended: April 7, 1997

Date: November 14, 2001

Revision: 9

A. Parties

The project was a relationship among LLNL, Los Alamos National Laboratory, Sandia National Laboratories, Oak Ridge National Laboratory and the industrial partner, The National Center of Manufacturing Sciences (NCMS).

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B. Project Scope

This project was a multi-lab, multi-partner CRADA involving LLNL, Los Alamos National Laboratory, Sandia National Laboratories, Oak Ridge National Laboratory, Martin Marietta Energy Systems and the industrial partner, The National Center of Manufacturing Sciences (NCMS). A number of member companies of NCMS participated including General Motors Corporation, Ford Motor Company, The Torrington Company, Gear Research, the Illinois Institute of Technology Research Institute, and Deformation Control Technology. LLNL was the lead laboratory for

metrology technology used for validation of the computational tool/methodology. LLNL was also the lead laboratory for the development of the software user interface for the computational tool. This report focuses on the participation of LLNL and NCMS.

The purpose of the project was to develop a computational tool/methodology that engineers would use to predict the effects of heat treatment on the size and shape of industrial parts made of quench hardenable alloys. Initially, the target application of the tool was gears for automotive power trains.

C. Technical Accomplishments

The major LLNL technical accomplishments fell into three broad categories:

1. Precision measurement of quench-induced distortions for various helical gear geometries and gear blanks, for a variety of processing conditions. This data was used to guide model development and as a validation of the end product computational tool. LLNL took a leading role in overall project quality assurance for the integrated system methodology.
2. Development of a coordinate measurement/computational model interface to enable accurate model verification. A software interface was developed to enable the complex three dimensional distortion measurement data to be compared directly to numerical simulations of distortions.
3. Development of a simplified, integrated, user interface that isolates a non-expert user from many of the complex details of setting up and running a numerical analysis with the sophisticated material model that was developed. This interface integrated automatic meshing of a broad class of part geometries, pulled in material properties and boundary conditions for different quench processes from an external database, and arranged and executed the multi-step analysis. LLNL led this effort, and the timely delivery of a working prototype (which was developed entirely at LLNL) was credited by the partners with saving the project from an untimely termination at a critical early project evaluation point.

LLNL completed the following aspects of the project:

- Measurement requirements document
- Conceptual design of gear measurement
- Quality assurance Plan
- Detailed design of gear measurement
- Measurement System Demonstration
- Metrology post processor /user interface operational
- User manual for the user interface
- Summary report on metrology measurements

Additional Accomplishments included:

- Developed detailed metrology measurement requirements plan
- Developed quality assurance plan
- Developed gear metrology software (QUINDOS)
- Performed precision metrology measurements on large number of parts:
 - Gear Research gear study
 - Equipment/Processing Task Team's study (>75 parts)
 - Taguchi based study on Gear Research gears (>40 parts)
 - Saturn gears and gear blanks for validation data (24 parts)
- Developed GUI tool to enable metrology distortion data to be compared with numerical simulations
- Designed overall software architecture of the "engineering tool" being developed as the major deliverable of this CRADA
 - Led effort at developing the user interface for the "software tool"
 - Designed and implemented the first working prototype
 - Provided updated software distribution to developers through our web-site
 - Wrote draft version of the online documentation of the software user interface
- Delivered a special version of the LLNL code TOPAZ to Ford to perform inverse heat transfer calculations.

Since the original milestones were proposed in 1992 before the project got underway, knowledge learned as the project evolved naturally led to some change in focus. There was some change in emphasis away from LLNL's originally proposed activities in materials characterization and independent code implementation and verification, towards much heavier than planned activities in gear metrology experiments (many more parts were measured than were originally planned for), as well as heavy involvement with development of the software user interface (an activity that wasn't originally identified, but ultimately became a major task). These changes in focus, and associated modifications in deliverables, were done in concurrence with and at the behest of the industrial partners.

The significant cutback in FY96 funds essentially eliminated LLNL's activities in materials characterization for the project. As a consequence, associated deliverables were dropped from Phase I of this project (with the concurrence of the industrial partners). Phase I ended up focusing on a single material system (5120 Steel) and ORNL was able to provide adequate materials testing to characterize the project material.

Also, the deliverable to compare ABAQUS calculations with independent code was limited to an early comparison with the HEARTS code. The decision to postpone implementation of the constitutive model into other codes until Phase II of this project was made in conjunction with the industrial partners.

LLNL delivered an approximately 90 page final report of our experimental results and in April 1997.

LLNL's milestones/deliverables (from original Project Task Statement):

Measurement requirements documents	Completed 7/94
Prototype design of gear measurement	Completed 9/94
Quality assurance plan	Completed 6/95
Enhanced Prototype design of gear measurement	Completed 3/95
Post processor operational	Completed 6/95
Measurement system demonstration	Completed 9/95
Report on comparison of part measurements and numerical calculations.	Report on measurements completed 4/97. Comparison with numer. calcs not done in Phase 1

Additional deliverables addressed after change in focus with partner consent:

Developed prototype of software tool user interface.	Completed 9/94
Completed user interface for Phase 1 software tool.	Completed 9/96
Developed online documentation for the software tool / user interface.	Completed 9/96.
Developed and maintained website enabling distribution of user interface, constitutive model (UMAT), data, etc. to project participants.	Activated 3/95
Measured of Saturn gears and gear blanks for validation data.	Completed 8/96

Milestones in the original plan that were dropped with partner consent (see above discussion):

- Variable temperature testing of 5120 alloy steel.
- Variable temp. testing of higher carbon steel.
- Report on independent assessment of ABAQUS calculations.
- Report on comparison of ABAQUS calc. with independent code.
- Report on independent assessment of constitutive equations.
- Variable temperature testing of "ideal" material.

D. Expected Economic Impact

In the metal-manufacturing industry, time and resources are lost dealing with the geometric distortion caused by heat treatment. Types of losses include direct scrap wastage caused by unanticipated changes in part shape, time, and cost involved in redesign iterations, higher capital costs for equipment to refinish out-of-tolerance parts, higher per piece production costs, and market deterioration caused by lengthened time-to-market. A tool that would effectively predict part distortion could significantly reduce these problems for the National Center for Manufacturing Sciences (NCMS).

The engineering analysis tools, materials characterization capabilities, and geometry measurement capabilities developed in the CRADA could be an asset to DOE nuclear weapons manufacturing operations, particularly in view of the complex modernization currently underway. Of the hundreds of unique components contained in typical nuclear weapons systems, most of the wrought metal parts undergo heat treatment or welding. These processes induce residual stresses and distortion. With only a few exceptions, DOE contractors have not successfully applied computational modeling to effectively predict these effects in nuclear weapons manufacture. This CRADA could consolidate DOE's expertise with that of the NCMS/Member Companies and other DP Labs to create a capability that would serve future DOE production needs, particularly as resources available to support production are reduced. The computational tool could also capture the technology for design and fabrication of heat-treated metal parts that would otherwise diminish as we lose the trial-and-error experience base that enabled DOE contractors to successfully produce parts.

D.1 Specific Benefits

Significant strides were made in the ability to model a thermo-mechanical process in which a solid material undergoes a solid-state change of phase, which accurately captured the phase transformation kinetics. The project also addressed modeling the effect of interstitial elements such as the effect of carburizing steel parts. This required the development of an extremely complex material model that pushed the boundaries of the state of the art. The metrology measurements used for validation required the development of the most complex control routines our Lab has had to deal with and has enhanced our internal capabilities.

E. Partner Contribution

NCMS/GM/Ford completed these aspects of the CRADA:

- Provided an evaluation of the HEARTS-2D (or -3D) code with all documentation, software, and licensing permission to use the software at the facilities in Oak Ridge, Tennessee.

- Provided gears for use in the Round Robin residual stress measurement effort
- Provided gears for the quenchant property study for use in the quenching experiments at a GM gear production facility
- Provided mid-chemistry range 5120 alloy steel stock with appropriate heat treatments for characterization efforts
- Provided mid-chemistry range higher carbon version of the 5120 alloy steel stock with appropriate heat treatments.

There was no further development or invention based on the software developed in this project.

F. Documents/Reference List

Reports and Technical Papers

1. "Predictive Model and Methodology for Heat Treatment Distortion — Phase 1 Project Summary Report," NCMS, Publication Date: September 30, 1997.
2. "Metrology Task Team Final Report," Nikkel, Daniel J., Jr., April 3, 1997.
3. "Predictive Model and Methodology for Heat Treatment Distortion — Metrology Task Team Phase 1A Report," September 27, 1994.
4. "Development of a Carburizing and Quenching Simulation Tool: Numerical Simulations of Rings and Gears," with Charles Anderson, Peggy Goldman, Partha Rangaswamy, Gregory Petrus, Lynn Ferguson, Jim Lathrop, Janis Keeney, Myron McKenzie, and Nagendra Palle, presented at the 2nd International Conference on Quenching and the Control of Distortion, Cleveland, OH, November 4-7, 1996.
5. "Development of a Carburizing and Quenching Simulation Tool: A Material Model for Low Carbon Steels Undergoing Phase transformations" D.J. Bammann, V.C. Prantil, A.A. Lamar, J.F. Lathrop, D.A. Mosher, Sandia National Laboratory; M. Lusk, H.J. Jou, G. Krauss, Colorado School of Mines; W. H. Elliott, Jr., Oak Ridge National Laboratory; d. J. Nikkel, Jr., Lawrence Livermore National Laboratory. Publication Date: July 1996
6. "Numerical Modeling of the Mechanics of Solid/Solid Phase Transformations," Anderson, C. Society of Engineering Science Annual Meeting. October 20-23, 1996.

7. "Development of a Carburizing and Quenching Simulation Tool: Numerical Simulations of Rings and Gears," Anderson, C., P. Goldman, P. Rangaswamy, G. Petrus, B. L. Ferguson, D. Nikkel, J. Lathrop, J. Keeney, G. Aramayo, M. McKenzie, and N. Palle. 2nd International Conference on Quenching and Distortion. November 4-7, 1996.
8. "A Model of Phase Transformation Plasticity," Bammann, D., V. Prantil, and J. Lathrop. ASME Materials and Mechanics Conference. June 11-14, 1995. Baltimore, Maryland.
9. "A Plasticity Model for Materials Undergoing Phase Transformations," Bammann, D., V. Prantil, and J. Lathrop. Engineering Science Foundation Casting and Welding Conference. September 11-14, 1995. London, England.
10. "Development of a Carburizing and Quenching Simulation Tool: A Material Model for Carburizing Steels Undergoing Phase Transformations," Bammann, D., V. Prantil, A. Kumar, J. Lathrop, D. Mosher, M. Callabresi, M. Lusk, G. Krauss, H. J. Jou, W. Elliott, G. M. Ludtka, W. E. Dowling, D. Nikkel, T. Lowe, and D. Shick. 2nd International Conference on Quenching and Distortion. November 4-7, 1996.
11. "Complementary Neutron and X-Ray Profiles Through a Carburized Surface," Bourke, M. A. M., P. Rangaswamy, and T. M. Holden. *Journal of Material Science Engineering* (1996).
12. "Development of a Carburizing and Quenching Simulation Tool: Program Overview," Dowling, W. E., B. L. Ferguson, Y. H. Gu, T. Pattok, D. Shick, and M. Howes. 2nd International Conference on Quenching and Distortion. November 4-7, 1996.
13. "A Coupled Model of Diffusive Phase Transformation," Lusk, M., G. Krauss, and H. J. Jou. *ASM Materials Week* (October 31, 1995).
14. "A New Balance Principle for Modeling Phase Transformation Kinetics," Lusk, M., G. Krauss, and H. J. Jou. International Conference on Martensitic Transformations (ICOMA T '95). August 15, 1995.
15. "Residual Stress and Microstructural Characterization Using Rietveld Refinement of a Carburized Layer in a 5120 Steel," Rangaswamy, P., M. Bourke, A.C. Lawson, J. O'Rourke, and J. A. Goldman. Advances in X-Ray Analysis Conference. August 6-8, 1995. Colorado Springs, Colorado.

16. "Experimental Measurements and Numerical Simulation of Stress and Microstructure in a Carburized 5120 Steel," Rangaswamy, P., M. Bourke, J. Shipley, and J. A. Goldman. Conference on Carburizing and Nitriding with Atmospheres. December 7, 1997. Cleveland, Ohio.
17. "Development of a Carburizing and Quenching Simulation Tool: Determination of Heat Transfer Boundary Conditions in Salt," Shick, D., D. R. Chenoweth, N. Palle, C. Mack, W. Copple, W. T. Lee, W. Elliott, J. Park, G. M. Ludtka, R. Lenarduzzi, and W. Walton. 2nd International Conference on Quenching and Control of Distortion. November 4-7, 1996.

Copyright Activity

Computer Software:

A computational tool (software) was developed as a part of this project. The software subsequently evolved into a product that is now called "Dante". The software consists of a variety of customized applications developed using commercial software, which are integrated under a common graphical user interface. The tool consists of: the user interface which handles the automated meshing, and analysis problem definition, execution and post-processing, was built with MSC/Patran®; material properties and boundary condition databases used in analysis problem definition were developed in M/VISION™; and the material constitutive model for use during the analysis execution was developed as an ABAQUS® UMAT. The software was jointly developed between laboratories and industrial partners, with the labs taking the leadership role and doing the majority of the initial work. LLNL was the lead laboratory in the development of the user interface and wrote a significant portion of the code. Contributions to development of the user interface were also made by LANL and Deformation Control Technology. Sandia was the principal developer of the material model (UMAT) with the transformation kinetics code being developed by the Colorado School of Mines.

Computer Software developed by LLNL:

QUINDOS program for measuring helical gears and gear blanks on the Leitz coordinate measuring machine. See also above.

Special version of the heat transfer code TOPAZ used for inverse heat transfer calculations to determine boundary conditions for quench analysis.

Computer Software developed by NCMS or Member Companies:

This CRADA does not require or provide for submission of copyrighted computer software to DOE's Energy Science and Technology Software Center.

Licensing Status:

The industrial partners plan to commercialize the software developed under this CRADA. Licensing was addressed in the CRADA, and the parties do not intend at this time to enter into a separate licensing agreement for the software commercialization. Sandia Laboratory is taking the lead in interacting with NCMS for such issues as revenue shares and distribution.

Subject Inventions:

LLNL Inventions:

None

NCMS and Member Company Inventions:

None

Joint Inventions:

None

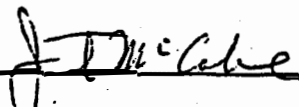
Background Intellectual Property

None

G. Acknowledgement

Participant's signature of the final report indicates the following:

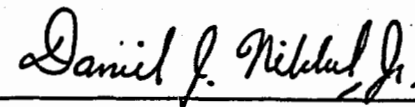
- 1) The Participant has reviewed the final report and concurs with the statements made therein.
- 2) The Participant agrees that any modifications or changes from the initial proposal were discussed and agreed to during the term of the project.
- 3) The Participant certifies that all reports either completed or in process are listed and all subject inventions and the associated intellectual property protection measures generated by his/her respective company and attributable to the project have been disclosed and included in Section E or are included on a list attached to this report.
- 4) The Participant certifies that if tangible personal property was exchanged during the agreement, all has either been returned to the initial custodian or transferred permanently.
- 5) The Participant certifies that proprietary information has been returned or destroyed by LLNL.



Jack McCabe
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12/06/01

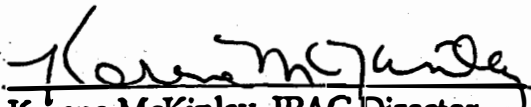
Date



Dr. Daniel J. Nikkel, Jr.
Lawrence Livermore National Laboratory

12/19/01

Date



Karena McKinley, IPAC Director
Lawrence Livermore National Laboratory

1/8/02

Date

Attachment I - Final Abstract

Predictive Model and Methodology for Heat Treatment Distortion

Final Abstract (Attachment I)

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B. Benefit to Industry

In the metal-manufacturing industry, time and resources are lost dealing with the geometric distortion caused by heat treatment. Types of losses include direct scrap wastage caused by unanticipated changes in part shape, time, and cost involved in redesign iterations, higher capital costs for equipment to refinish out-of-tolerance parts, higher per piece production costs, and market deterioration caused by lengthened time-to-market. A tool that would effectively predict part distortion could significantly reduce these problems for the National Center for Manufacturing Sciences (NCMS).

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D. Dates of Project

January 1994– April 7, 1997