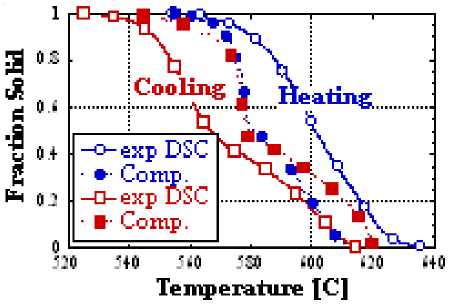
Industrial Technologies Program

Inverse Process Analysis for the Acquisition of Thermophysical Data

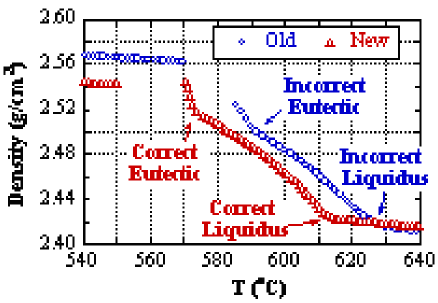
Increased Accuracy of Thermophysical Materials Properties Data and More Accurate Simulations Will Lead to Improvements in Materials Processing

One of the main barriers in the analysis and design of materials processing and industrial applications is the lack of accurate experimental data on the thermophysical properties of materials. To date, the measurement of most of these high-temperature thermophysical properties has often been plagued by temperature lags that are inherent in measurement techniques. These lags can be accounted for with appropriate mathematical models, reflecting the experimental apparatus and sample region, in order to deduce the desired measurement as a function of true sample temperature.

Differential scanning calorimeter (DSC) measurements are routinely used to determine enthalpies of phase change, phase transition temperatures, glass transition temperatures, and heat capacities. DSC data have also been used to estimate the fractional latent heat release during phase changes. In the aluminum, steel, and metal casting industries, predicting the formation of defects such as shrinkage voids, microporosity, and macrosegregation is limited by the data available on fraction solid and density evolution during solidification. Dilatometer measurements are routinely used to determine the density of a sample at various temperatures. An accurate determination of the thermophysical properties of materials is needed to achieve accuracy in the numerical simulations used to improve or design new material processes.



The computed fraction solid for alloy A356 using the current DSC model



Comparison of dilatometer results obtained with the new and old setup

Benefits for Our Industry and Our Nation

The benefits of obtaining accurate materials properties involving both thermal and mechanical character include:

- *Total manufacturing industry cost savings of $94 million/year by the year 2020.*
- *Total manufacturing industry energy savings of 17 TBtu/year by the year 2020.*
- *Environmental savings of 236 thousand tons of CO_2/year and 2.05 thousand tons of NO_x/year by the year 2020.*

Applications in Our Nation's Industry

Accurate thermophysical properties are necessary for a wide application base and thus are inherently crosscutting in nature. Several industries will derive benefits from this investigation, including:

- Aluminum
- Glass
- Metalcasting
- Steel

Project Description

The goal of this project was to extend the utility, quality and accuracy of two types of commercial instruments — a differential scanning calorimeter (DSC) and a dilatometer — used for thermophysical property measurements in high-temperature environments. In particular, the quantification of solid fraction and density during solidification was deemed of critical importance. To accomplish this project goal, sample holders were redesigned and inverse mathematical methods were developed to account for system lags. The desired property could then be correlated to the proper sample temperature based on using remote temperature measurements.

Barriers

- In current state-of-the-art, high-temperature thermophysical property measurement tools, time lags are inherent because:
  - a) The sample temperature cannot usually be measured directly and the temperature data are recorded by using a thermocouple that is normally placed at a different location from the sample's location, and
  - b) There is a nonhomogeneous temperature distribution within the instruments themselves.

Pathways

- The thermal lag can be estimated and its effect can be taken into account in determining the desired thermophysical properties by performing a computational analysis of the measurement process
- In order to describe the DSC system with minimal components, an analysis was performed to ascertain the effect of each of the components
- An alternative direct approach to the inverse method was developed in order to determine the enthalpy and ensuing distribution of the solid fraction during solidification
- For the dilatometer, the sample holder was redesigned and inverse mathematical methods were developed to account for system lags

Results

- The DSC heat transfer model was validated for pure aluminum and successfully applied to a study of the commercial aluminum alloy A356
- Dilatometer temperature error has been reduced from ±30°C to approximately ±6°C at temperatures of 600-700°C
- This project has led to very accurate solid fraction data measurements with ±3% error and reduced the temperature error for improved density measurements to ±0.5°C

Commercialization

This project was a feasibility study. The algorithm developed for establishing sample temperature in the DSC and the newly designed sample holder with inverse analysis for the dilatometer present two potential products for measurement device manufacturers. The dissemination of the findings in conference and archival publications provides opportunities for readers to contact Oak Ridge National Laboratory (ORNL) and the University of Tennessee at Knoxville (UTK).

As an additional opportunity to validate the results of the modeling and improved experimental procedures determined from this project, the computational approach was utilized in another project, "Predicting Pattern Tooling and Casting Dimensions for Investment Casting" (DE-FC36-01ID14003), in order to obtain optimal thermophysical properties for aluminum alloy A356. NETZSCH, Inc., one of the instrument manufacturers, expressed interest in the results of this project.

Project Partners

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ESI, Inc.

A Strong Energy Portfolio for a Strong America

Energy efficiency and clean, renewable energy will mean a stronger economy, a cleaner environment, and greater energy independence for America. Working with a wide array of state, community, industry, and university partners, the U.S. Department of Energy's Office of Energy Efficiency and Renewable Energy invests in a diverse portfolio of energy technologies.

U.S. Department of Energy
Energy Efficiency
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