

## **(18) Preventing Solidification Defects in Large Superalloy Castings Used in Advance Electric power Systems**

This two-year effort will study macrosegregation in superalloy remelting processes. Weaknesses in existing models, particularly the inability to accurately predict partition coefficients of key elements under real operating conditions, will be addressed. Compositional effects of individual alloying elements in different alloys will be characterized so that a comprehensive database will be available in a useable format. A predictive methodology incorporating advanced computation technologies will be developed. Alloy index of freckle and center segregation formation can be determined for complex alloy compositions with efficient computational and laboratory analysis. The ultimate goal is to develop a predictive technology that can be applied commercially to prevent solidification defects for large superalloy castings used in advance electric power systems.

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Project Lead: West Virginia Research Corp. on behalf of West Virginia University

Project Participants: GE Energy; Special metals Corp.; Pennsylvania State University

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### Presentations/Publications

None.

### Patents

None.

### Progress in Past Quarter and Current Status

#### **Task 1: Solidification Modeling**

##### **Task 1.1 Thermodynamics Database and Partition Coefficients**

##### **Sub-task 1.1.1 Thermodynamic Modeling (Liu/PSU)**

*\*Tables and figures from the original report could not be pasted into this report. They are available for review upon request.*

The goal for this subtask is to obtain the partition coefficient of the model systems Ni-Cr-Nb, Ni-Cr-Fe, Ni-Cr-Ti, Ni-Cr-Fe-Nb, and Ni-base superalloys IN 706 & IN 718, through first-principle calculation and thermodynamic modeling. During the second quarter, the research efforts were focused on studying the methods to predict the partition coefficients of alloying elements by considering the thermodynamic and/or kinetic effects. They include,

- (i) the equilibrium calculation, at each temperature both solid and liquid phases are in thermodynamic equilibria, i.e. the diffusions of alloying elements in the liquid and solid phases are assumed to be infinitely fast;
- (ii) the Scheil model, there are infinitely fast diffusions of all alloying elements in the liquid and no diffusions in the solid;
- (iii) the kinetic simulation (by Dictra), the diffusions of alloying elements in the solid phase (the so-called back diffusions) and the liquid phase are not infinitely fast. The Thermo-Calc and Dictra codes [1] are used to study the above methods (i), (ii) and method

(iii), respectively. A model alloy Ni-15Cr-4.5Nb (in weight percent) is chosen to study the effects of different simulation methods on the partition coefficients of Cr and Nb. The influence of Nb content on the partition coefficients of Cr and Nb in Ni-15Cr-xNb alloys is also studied. The used thermodynamic data are taken from the recent assessment [2], the used kinetic data are taken from the NIST mobility database.

#### (1) The influence of different methods on partition coefficients

During the simulation, only the liquid and solid (fcc) phases in Ni-15Cr-xNb alloys are considered. For the diffusion controlled phase transformation simulated by Dictra, the cooling rate 1 K/s is employed. The calculated solid fraction of Ni-15Cr-4.5Nb as a function of temperature is shown in Fig. 1. The predicted partition coefficients of Cr and Nb in Ni-15Cr-4.5Nb as a function of solid fraction are illustrated in Fig. 2.

For solid fraction less than 0.5, Figs. 1 and 2 show that there are no obvious differences among the predicted properties by the three kinds of simulations: equilibrium calculation, Scheil model and Dictra simulation. The considerable differences among the three kinds of simulations appear when solid fraction greater than 0.5. The Dictra results (cooling rate 1 K/s) are located in the middle of the results obtained by equilibrium calculation and Scheil model, and close to those of the Scheil model. It is believed that the realized solidification is between the two extreme conditions: one is the complete diffusion in solid (equilibrium solidification), the other one is no diffusion in solid (Scheil model). Therefore the results from the Dictra simulation should be close to the realized condition.

Fig. 1 shows that the solid plus liquid region is only 30 K for Ni-15Cr-4.5Nb under equilibrium condition, while the Dictra simulation, especially the Scheil model, predicts that the solidification takes place in a temperature range over 100 K. Fig. 2 shows that the partition coefficients of Cr and Nb increase with increasing of solid fraction. When solid fraction is greater than 0.8, both Dictra and Scheil simulations indicate that the increasing of partition coefficient of Nb is much faster than that of Cr. When the solid fraction is closer to 1, the partition coefficient of Cr shows a decreasing trend predicted both by Dictra simulation and Scheil model. Fig. 2 also indicates that the partition coefficient of Nb depends greatly on the solidification conditions, such as the cooling rate, when the solid fraction is close to 1.

#### (2) The influence of Nb content on partition coefficients

The influences of Nb content on the temperature vs. solid fraction curves, and the partition coefficients of Cr and Nb in Ni-15Cr-xNb as a function of solid fraction, are shown in Figs. 3 and 4 for the equilibrium calculation, respectively. Figs. 5 and 6 are results for Scheil model. Figs. 7 and 8 are results for Dictra simulation with cooling rate 1 K/s. With increasing of Nb content, three kinds of simulations indicate that the phase transformation temperature decreases while the partition coefficients of Cr and Nb increases for each fixed solid fraction. As mentioned in the above section and indicated by Figs. 5 to 8, the results obtained from Scheil model and Dictra simulation are close to each other.

In summary of subtask 1.1.1, the partition coefficients of Cr and Nb in a model alloy Ni-15Cr-4.5Nb (in weight percent) are studied by using three kinds of simulation methods, (i) the equilibrium calculation; (ii) the Scheil model and (iii) the Dictra simulation. It is found that the partition coefficients predicted by Dictra simulation (cooling rate 1 K/s) are located in the middle of the results of equilibrium calculation and Scheil model, and close to those of Scheil model. With increasing of Nb content, the phase transformation temperature decreases while the partition coefficients of Cr and Nb in alloy Ni-15Cr-xNb increase for each fixed solid fraction.

### **Sub-task 1.1.2 Experimental Investigation on Partition Coefficients (Liu/WVU)**

The objective of this subtask is to experimentally study the solidification characteristics of Inconel 706, Inconel 718, and several model Nb, or Ti-content alloys. The solidification characteristics include partition coefficient, liquid composition, core dendrite composition, and liquid fraction as the function of temperature. The experimental outcome will be used to calibrate thermodynamic calculations.

During the second quarter of the project, the research efforts were focused on preparing the alloy samples, and determining their solidus and liquidus temperatures using differential thermal analysis.

These experimentally found liquidus and solidus transition temperatures will serve to design the experimental procedures for modified DTA quenching tests aiming to study the mentioned solidification characteristics as function of temperature.

#### **(1) Production of Model alloys using Arc bottom Furnace**

The tri-arc button furnace intended to prepare the model alloys was hooked up after obtaining the missing parts. Technical difficulties associated to the operation procedure of the furnace were encountered while performing the trial runs. Consumable supplies and replacement of parts were needed before the development of know how skills and obtaining control over the arc.

From the analysis of the raw EDS data, it was observed that the chemical composition was almost the same everywhere, which means that the procedure of three steps of melting for each sample was appropriate to thoroughly mixing the components. The EDAX results of these alloys are listed in Appendix I.

#### **(2) DTA Measurements of Phase Diagrams**

Differential Thermal Analysis (DTA) was used to study the phase diagrams of all the model alloys prepared. Three runs were performed for every sample, and the temperatures of solidus and liquidus transitions were averaged from the recorded values during melting and solidification on each run and between different runs.

All experiments were performed using a heating and cooling rate of 10°C/min, and Argon was used to purge the furnace and prevent oxidation of the samples. The maximum heating temperature of the tests is 1550°C. The DTA curves for each sample are listed in Appendix II.

From comparison between the theoretical transformation lines and the tendency lines corresponding to the experimental values, it was apparent that the measured values of Ni-20Cr-Nb alloys are similar to those obtained by theoretical calculation, but the measured values of Ni-15Cr-Nb are higher than Thermo-Calc results. It should be pointed out that the experimental liquidus and solidus values used in the comparison are the ones obtained by taking average of heating and cooling values; therefore the heating rate effects should be eliminated. Therefore, the gap between theoretical and experimental results could be attributed to the inaccuracy of the thermodynamic database associated with the Thermo-calc software, which was the center hypothesis of this project. It can be concluded that more *ab initio* calculations on the thermodynamic properties of Ni-Cr-Nb alloy system are needed to obtain accurate phase diagram of these alloys.

### **Task 2 Directional Solidification Verification**

The goal of this task is to experimentally study the effects of composition and kinetic parameters during solidification on the formation of macrosegregation defects, especially freckles. A

directional solidification (DS) furnace will be built and employed in the investigations.

#### **Task 2.1 Verification of Model Alloys (Liu/WVU)**

The objective of this task is to carry out DS of a series of simplified alloys with various eutectic phases, such as Laves phase,  $\delta$ -Ni<sub>3</sub>Nb, or  $\eta$ -Ni<sub>3</sub>Ti, to verify and modify phase diagram database and solidification modeling. During the second quarter, the research effort was focused on bringing the directional solidification furnace to operational state.

Drawings and technical specifications were obtained from the manufacturer, and it was found that the original design of the DS furnace requires an electrical power supply of single phase 115 Volts at 60 Amps. Due to high losses of power because of joules heating effects on the wiring systems, this kind of power supply is not found commonly in University facilities.

After studying the wiring layouts of the furnace and the controller, a practical solution to this difficulty was proposed. It consists on taking advantage that the furnace has three heating zones, controlled independently, and connect each of these heating zones to different phase lines and converting the single phase 115 Volts at 60 Amps to a three phase 115 volts at 20 Amps each. Currently the feasibility of the proposed modification, using the original controller, is being explored.

It was found also that the DS furnace is lacking of the specimen ceramic tray and heart thermocouple. These two parts are being quoted and the first experimental runs will be performed when these parts arrive.

#### **Plan for Next Quarter:**

##### **Task 1: Solidification Modeling**

##### **Task 1.1 Thermodynamics Database and Partition Coefficients**

##### **Sub-task 1.1.1 Thermodynamic Modeling (Liu/PSU)**

In the next quarter, the partition coefficient of the model systems Ni-Cr-Nb, Ni-Cr-Fe, Ni-Cr-Ti, Ni-Cr-Fe-Nb will be investigated, including

- (i) the effect of different databases on the partition coefficients;
- (ii) the effect of alloying elements on the partition coefficients;
- (iii) the effect of solidification conditions (such as cooling rate, back-diffusion) on the partition coefficients;
- (iv) Interpretation of available partition coefficients measured by taking back-diffusion into account.

##### **Sub-task 1.1.2 Experimental Investigation on Partition Coefficients (Liu/WVU)**

The research effort of the next quarter will be to develop the following activities:

- a. Obtain control over the final chemical composition of the model alloys.
- b. Produce the complete set of model alloys listed in table I.
- c. Determining the liquidus and solidus transitions for all the model samples prepared.
- d. Modify DTA machine for quenching.
- e. Perform Modified DTA runs and calculate partition coefficients from direct measurements of core dendrite and liquid composition
- f. Defining the next batch of experimental alloys

##### **Sub-task 1.1.3 Kinetic Effects**

The partition coefficients and other solidification characteristics of the first batch (Ni-Cr-Fe-Nb) of alloys will be investigated under various heating and cooling rates to study the kinetic effects on solidification behaviors of these alloys.

#### **Task 2 Directional Solidification Verification**

##### **Task 2.1 Verification of Model Alloys (Liu/WVU)**

The research effort of the next quarter will focus on bring to operational state the DS furnace and run the first experiments, using the batch of alloys defined in table I, under different rates of cooling.

**Task 2.2 Effect of Processing Parameters**

The research team will decide the experimental plan on the investigation of processing parameter effect, based on results of tasks 1.1.1 through 1.1.3. The experiments are expected to start from the third quarter of the project.

**References**

- 1 J. O. Andersson, T. Helander, L. H. Hoglund, P. F. Shi and B. Sundman, *Calphad*, **26** (2002) 273-312.
- 2 Y. Du, S. H. Liu, Y. A. Chang and Y. Yang, *Calphad*, **29** (2005) 140-148.