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**DEVELOPMENT OF A NEAR-NET-SHAPE
CASTING TECHNOLOGY FOR THE U-6Nb ALLOY—PART I: MATERIALS
CHARACTERIZATION, EXPERIMENT DESIGN, AND MODEL CONSTRUCTION¹**

M. J. Taylor,* E. L. Bird,** A. L. Demint,** J. A. Keeney,* and M. W. Wendel*

*Oak Ridge National Laboratory²
Lockheed Martin Energy Research Corp.

**Oak Ridge Y-12 Plant³
Lockheed Martin Energy Systems, Inc.

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ABSTRACT

The Oak Ridge Y-12 Plant (Y-12) is conducting highly coupled experimental and numerical studies to develop the technology needed to produce near-net-shape (NNS)-cast uranium-6 wt% niobium (U-6Nb) components which have a controlled carbon content. Current activities are focused on defining mechanical and metallurgical properties of cast material; experimental studies to define NNS casting, carbide particle flotation, and immersion-quench physics; and developing the numerical models needed to support the optimized design of NNS components. This paper summarizes the material characterization, experiment design, and model development activities.

INTRODUCTION AND GENERAL PROBLEM STATEMENT

MASTER

Y-12 produces uranium (U) and uranium alloy castings using graphite molds as a part of its production activities. In response to increased environmental concerns over the handling of uranium wastes, Y-12 is investigating new production techniques which have the potential to significantly reduce these wastes. Two such concepts are replacing the existing wrought process for producing parts with a casting procedure and increasing the use of recycled wastes as feed material. These processes have two potential advantages: (1) cast parts could be near-net shaped, thus reducing the total required feed; and (2) additional wastes could be recycled, further reducing the plant's waste stream. Extensive recycling, however, causes an accumulation of carbon, which can have deleterious effects on material properties. The carbon-removal technique chosen for initial evaluation involves adding trace amounts of an alloying agent to combine with

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the carbon. The resulting compound will be less dense than liquid U-6Nb, so buoyancy forces will transport it toward the top of the casting, where the carbon-rich portion can be removed after solidification. Determining the technical feasibility of these coupled processes requires an understanding of casting and metallurgical physics as well as the overall NNS-casting/waste-recycle (NNSC/WR) process.

The NNSC/WR process will attempt to use much higher amounts of recycled stock and will replace the current labor-intensive 19-step wrought process with three basic steps: (1) an NNS casting, (2) a heat-soak and immersion quench, and (3) final machining. Additionally, numerical models will be required to support design-optimization studies. The number of process unknowns in this problem definition are extensive:

1. Most significant is the metallurgical acceptability of cast U-6Nb. It is not certain that cast parts produced even from virgin U-6Nb will meet the strict quality criteria of wrought parts.
2. Casting will use vacuum-induction furnaces. The effects of induction heaters on mold temperatures and of magnetic fields on fluid convective currents are unknown.
3. Requiring a specific microstructure within an NNS part means that heat conduction in the mold could be a controlling mechanism. Values for typical thermal resistances, especially the melt/mold-interface heat-transfer coefficient, and their cumulative effects on microstructure are undefined.
4. Carbide-formation and -floatation physics are equally uncertain:
 - (a) Do carbides form in the crucible prior to the pour or after the pour during solidification?
 - (b) Which alloying agent maximizes flotation?
 - (c) Is it feasible to optimize both flotation and microstructure during solidification? These are potentially conflicting figures of merit, and it might be necessary to float out inclusions in a separate step.
 - (d) Will the upper surfaces of the mold obstruct flotation?
5. Some parts have surfaces with different orientations relative to gravity. This configuration results in a single part having different time- and position-dependent quench heat-transfer coefficients. These coefficients have a significant effect on residual stresses and deformation but are currently undefined and will have to be studied in detail.
6. The quench and machining steps will also influence the optimized NNSC/WR process. As the extent of near-net shaping is optimized, there is the potential for excessive deformation during quenching or machining. Thus, the cumulative effects of these steps must also be defined.
7. In addition to these problem-specific unknowns, there is the requirement to understand the effects of traditional casting variables such as heating-coil design and melt superheat on part quality.

Superimposed on these process considerations are uncertainties with data on U-6Nb properties. Macroscopically, U-6Nb has a shape-memory effect whose influence on dimensional stability during heating and machining is not well defined. Also, distortion can result from twinning; the relationship between this mechanism and metallurgical phase distributions is uncertain. As is the case for most uranium alloys, individual properties can be quite complex. For example: (1) solid and liquid thermophysical properties are temperature-dependent; (2) mechanical properties are strongly anisotropic as well as temperature-, phase-, and strain-rate-dependent; and (3) solid-state phase changes are complicated functions of time and temperature. These properties must be defined before accurate numerical models can be completely developed.

The feasibility of the NNSC/WR process therefore rests on essentially five considerations:

1. the ability to produce cast parts with acceptable properties using recycled material,
2. the ability to optimize NNS-cast parts without being overly constrained by quenching and machining,
3. the ability to float out carbide particles prior to or during casting,
4. the availability of numerical models with sufficient rigor to simulate NNSC/WR physics, and
5. the availability of adequate U-6Nb properties data.

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Coupled experimental and numerical studies are being implemented to address these concerns and develop a mature NNSC/WR technology. The goals are to define material properties of cast U-6Nb, define basic NNSC/WR physics, and develop the numerical models needed to optimize the design of NNSC/WR components. Because of the complexity of the problem, the scope of this current effort is limited to the casting and quenching steps. An additional simplification is that experimental studies conducted to define casting physics will use simplified geometries so that individual mechanisms can be somewhat isolated and studied in detail. Furthermore, modeling studies will utilize commercial software rather than newly constructed in-house codes. If commercial software can be shown to be adequate, then expensive in-house codes will not have to be developed to conduct design optimization studies. Also, modeling studies will use the best U-6Nb properties data currently available. While this approach might limit the early acquisition of physical insight, it will permit a systematic evaluation of the need for accurate properties. The remainder of this paper describes material-characterization, experiment design, and model-development activities.

MATERIALS CHARACTERIZATION OF CAST U-6Nb

Three nonoptimum-NNS U-6Nb parts were cast using vacuum-induction furnaces and 100% recycled material that contained approximately 115 ppm carbon. After casting and prior to quenching, the parts were degassed and had their outside surfaces slightly contoured. The quench consisted of two steps: a vacuum gamma-solution heat treatment and an immersion quench in water. After the quench, test specimens were removed from each part for tensile and metallographic examination. The parts were then machined to final dimensions and subjected to an extensive series of dimensional inspections, radiographs, and metallographic examinations.

Visual and Dimensional Inspections

Visual inspection of each part revealed no gross banding or segregational patterns that might be indicative of dendritic coring. Coordinate-measurement-machine (CMM) data were taken before and after the quench to determine dimensional accuracy and stability. Analysis of these data revealed the following results:

1. approximately 2% axial shrinkage and some loss of definition (i.e., thinout) on sharp-radius corners;
2. no significant change in part dimensions resulting from the quench.

Radiographic and Dye-Penetrant Examinations

Prequench and postmachining radiographs were made to determine if large voids or defects were present. At a resolution of 0.500 mm, two parts had no detectable cracks, voids, or inclusions. The third had 17 low-density areas, the largest being 1.651 x 1.142 mm with a radial depth of 0.625 mm. Although this part had no detectable cracks or inclusions, it was rejected using the wrought-part inspection criteria. Final machined parts were dye-penetrant inspected for surface defects, and all three parts were rejected. Innumerable dye indications were found. These flaws ranged from approximately 0.127 to 2.28 mm and were located primarily on the surface.

Metallographic Examinations

Specimens from each part were used to define mechanical properties, grain size, inclusions, and niobium segregation. Table 1 summarizes typical results from two specimens from each part. Follow-on scanning electron microscopy (SEM) examinations were conducted on those specimens with the lowest elongation values. This investigation revealed the presence of a large niobium-rich inclusion on the 2a specimen (lowest elongation) and much smaller uranium-rich inclusions on the 1a and 3b specimens. Fractographic analysis of the other specimens (i.e., nominal elongation values) revealed a heavily dimpled failure mode indicative of good ductility.

Table 1. Selected Mechanical Properties of NNSC/WR U-6Nb

Specimen	Tensile Strength (psi)	Yield Strength (0.2% O.S.) (psi)	Elongation in 0.64 in. (%)	Reduction in Area (%)	Modulus of Elasticity ($\times 10^6$ %)
NNSC 1a	121,600	24,400	18.8	19.0	9.9
NNSC 1b	124,500	24,300	29.7	30.7	9.9
NNSC 2a	95,500	25,900	4.7	7.4	10.0
NNSC 2b	124,500	24,800	29.7	28.6	10.0
NNSC 3a	126,400	29,000	28.1	31.1	9.9
NNSC 3b	127,900	27,000	21.9	20.0	10.0

Grain Size, Inclusions, and Niobium Segregation

Fig. 1 shows a photomicrograph of typical grain size. This rather large grain structure ranged from 10 to 400 μm , with an average size of approximately 150 μm . Table 2 summarizes the inclusion analysis and comparison data from vacuum-arc-melted (i.e., VAM, an intermediate step in the wrought process) material. The average number of oxides for all three parts was 54/ mm^2 and the number of oxides + carbides was 358/ mm^2 , indicating total carbides of 304/ mm^2 . The average niobium concentration in weight percent for all three parts was $5.68\% \pm 0.38\%$. Fig. 2 shows a typical niobium-segregation spectrum. This variation is slightly greater than typical wrought material but within specifications. Fig. 3 shows an X-ray image of the typical distribution of niobium, which is evenly disbursed with no evidence of macrosegregation.

Fig. 1. Typical grain structure for NNSC/WR material.**Table 2. Inclusion Analysis of NNSC/WR U-6Nb**

	Part #1	Part #2	Part #3	VAM
Oxides				
Total found	40	70	115	NA
Minimum area, μm^2	2	2	2	NA
Maximum area, μm^2	12	8	3	200
Mean area, μm^2	4	3	6	6
Average/ mm^2	29	51	83	50
Carbides plus oxides				
Total found	561	633	286	NA
Minimum area, μm^2	2	2	2	NA
Maximum area, μm^2	56	81	424	1179
Mean area, μm^2	10	10	22	35
Average/ mm^2	410	458	207	150
Number of inclusions 0 - 10 μm^2	506	579	208	170
10 - 100 μm^2	55	653	66	140
100 - 200 μm^2	0	0	9	20
>200 μm^2	0	0	1	2

Fig. 2. Typical niobium spectrum for NNSC/WR material.

Fig. 3. X-ray image of niobium inclusions for typical NNSC/WR material.

Discussion of Results

Prominent observations and interpretations of test results are as follows:

1. Gross banding or segregational patterns indicative of dendritic coring are not present in the NNSC/WR material. Although the niobium scatter is somewhat greater than in wrought material, the overall variation meets current specifications.
2. The 2% axial shrinkage will require that additional material be factored into future castings. The shrinkage (loss of definition) observed could restrict the ability to obtain a final-machined part, and this could pose a problem as component designs are driven toward NNS.
3. Distortion resulting from the heat-treat quench is not a problem but could become a concern as designs are driven toward NNS.
4. Grain sizes are not as uniform or as small as those found in wrought U-6Nb. The microstructure of NNSC/WR material consists of a mixture of relatively small grains or subgrains scattered throughout the matrix along with some very large grains.
5. Solution heat-treated and quenched NNSC/WR material is comparable to, possibly superior in strength to, but slightly lower in ductile properties than wrought U-6Nb.
6. Of most concern are the large numbers of surface flaws that caused the parts to fail the dye-penetrant test. The reasons for these imperfections are currently unknown. Preliminary SEM examination suggests a relationship between the flaws and inclusions.
7. The number of carbide inclusions appears to be three to four times greater than wrought U-6Nb but are of a much smaller size. Indeed, the number of inclusions greater than $100\text{ }\mu\text{m}^2$ is practically zero for the NNSC/WR material, whereas for the arc-melted material it is significantly higher. The average volume of oxides + carbides for the NNSC/WR material is almost the same as for the arc-melted material. Macroscopically, the larger total number of inclusions in the NNSC/WR material is consistent with using 100% recycled stock.

EXPERIMENT DESIGN AND INITIAL MODEL CONSTRUCTION

The specific goal of the casting studies is to acquire the physical and numerical insight needed to design a quench-constrained NNS mold and solidification transient which gives the carbon compounds time to float to the top of the casting but which also constrains the solidification time so that only the desired microstructures will form. The quench objective is similar: understand quench physics to the level required to calculate the optimum thickness that permits parts to be quenched without excessive deformation or residual stresses. The basic numerical issue to be studied is the required rigor of the models; that is, the minimum geometry, physics, and properties approximations required to obtain acceptable agreement with experimental data. Making this determination will simultaneously generate the required numerical insight and determine the acceptability of commercial software. Understandably, these objectives have as many computational uncertainties as process unknowns. Accordingly, an iterative highly coupled experimental-numerical development program was defined to simultaneously quantify NNSC/WR physics and develop the numerical models.

Quench Experimental Studies and Model Development

Predicting quench-induced distortion and residual stresses in a material with complex anisotropic material properties and solid-state phase changes requires solving a nonlinear coupled thermal/stress problem. Sophisticated commercial software exists for simulating these physics, and model development generally reduces to obtaining adequate material properties and thermal boundary conditions. Such is the case with the quench facet of the NNSC/WR problem. Given this degree of numerical sophistication, it will not be necessary to conduct an exhaustive series of experimental studies to characterize distortion as a function of part thickness. It will only be necessary to conduct those few tests needed to define generic model input and stress/distortion data at a single thickness for validating the model. This current study addresses only model input.

The generic input required for this problem (besides material properties) consists of the quench heat-transfer coefficients. Because boiling heat transfer is a surface phenomenon, coefficients defined for one thickness can be used for any other thickness, so long as they all have the same surface finish and orientation.

Quench System Description

A typical quench system consists of a large-diameter vacuum furnace which contains strip heaters and a removable bottom flange. The flange is connected to a hydraulic piston that extends down into the quench pool. The total distance from the bottom of the furnace to the water is about 10 ft. This overall configuration is shown in Fig. 4. The part to be quenched is positioned on the flange, the furnace sealed, and a vacuum established. The part is then slowly heated to the gamma range, about 800°C. After steady state has been established, argon is slowly vented into the furnace. Once the pressure reaches atmospheric pressure, the bottom flange is opened and the hydraulic piston lowers the flange with the part into the room-temperature water.

Fig. 4. Schematic illustration of typical quench facility.

Quench Experiment Design

The goal of the quench studies will be to define time- and position-dependent quench heat-transfer coefficients for typical parts. One or more parts with the same thicknesses will be cast, have their surfaces lightly contoured, and be dimensionally inspected. Buried thermocouples will be installed at those locations where different coefficients are expected. The instrumented parts will then be quenched once. Each experiment will generate transient temperature data as well as pre- and postquench dimensional inspection results. The temperature data will have to be reduced to define the coefficients, and this exercise will require considerable effort.

Heat-transfer coefficients will be calculated using two inverse heat-conduction techniques: a localized procedure and a whole-domain approach. Both approaches determine the surface heat flux required to give the measured temperature transient. The localized procedure calculates a heat-flux value for each time step in a transient, while the whole-domain approach calculates a function that describes heat flux for a complete transient. Y-12 has a validated computer program to conduct the localized analysis [Park and Ludtka, 1989], and the following briefly describes the whole-domain procedure and data-reduction computer programs to be constructed for this exercise.

The whole-domain analysis begins by assuming that a coefficient can be described by a relatively simple function such as

$$h = a + b \sin(T_s - c),$$

where a , b , and c are unknown constants and T_s is the measured surface temperature. Defining values for the constants is accomplished by (1) constructing a transient heat-conduction model of the thermocouple and a portion of the surroundings and (2) executing the model in an iterative sequence to determine values which minimize the difference between calculated and measured surface temperatures. The most important element in this sequence is an efficient iterative procedure. The approach to be used for this problem is based on the realization that determining the unknown coefficients is essentially an optimization problem, that is, determining the set of values for the unknown constants which minimizes the difference function. The HEATING computational heat conduction (CHC) code [Childs, 1991] will be used to construct the transient conduction model. The code will be modified to function as a subroutine and input to the GRG2 commercial optimization code [Lasdon and Warren, 1989]. GRG2 will then drive the model to determine the values. To date, HEATING has been modified and the GRG2 input routines have been written.

Both data-reduction techniques require the transient temperature data to be smoothed prior to the calculations. Accordingly, a FORTRAN program was constructed using the moving-window smoothing technique [Park and Ludtka, 1989]. This procedure replaces each transient data point with a value calculated from a least-squares curve fit. The curve fit uses actual data taken from an interval around the current point. The program constructed for this effort utilized a variable window size and four least-squares curve fits. Results showed that smoothing was unaffected by curve-fit type so long as the window was sufficiently large.

Both data-reduction techniques assume that parts have a uniform temperature just before immersion. This simplifies the analysis and permits one to calculate just the quench coefficients. Otherwise, data reduction would have to begin when the flange is first opened and determine separate drop and quench coefficients. This would increase the cost of the data-reduction exercise and the uncertainties associated with the quench coefficients. To verify this uniform-temperature assumption a coupled thermal/fluids study of a nominal geometry (i.e., not an actual part) was conducted using the CFX computational fluids dynamics (CFD) code [Computational Fluid Dynamics Service, 1995]. The analysis calculated natural- and forced-convection heat transfer from the part beginning when the furnace flange is opened and continuing until it just reaches the water. In addition, a separate one-dimensional calculation was made to estimate the additional energy loss due to radiation heat transfer. These calculations showed the temperature difference across the thickness of the part would be less than 5K. Thus, the simplifying assumption was justified. The problem geometry and typical CFX results are shown in Fig. 5.

Fig. 5. Typical CFX transient results showing streamlines around flange-part system just before immersion.

An additional problem-specific consideration is the scope of the data-reduction exercise. Separate coefficients will have to be defined for those part surfaces where different heat-transfer coefficients are expected; that is, those surfaces with different orientations relative to gravity. Part geometry further complicates the problem. The assumption usually made when constructing the conduction model is that all surfaces of a part will experience the same heat flux. This permits one to use a plane of symmetry in the conduction model. Given the potential for surfaces to have significantly different heat fluxes, this assumption is not justified. Thus, an iterative execution procedure will have to be developed where sets of coefficients are defined simultaneously.

Quench Model Construction

The ABAQUS/Standard commercial stress analysis code [Hibbitt, Karlson, and Sorensen, 1994] will be used to model quench-induced distortion and residual stresses. This selection was based on the code's ability to perform a coupled thermal/elastic-plastic stress analysis as a function of anisotropic mechanical properties, time- and temperature-dependent internal heat generation, and time- and position-dependent thermal boundary conditions. Execution will be divided into two phases, model validation and parametric studies to acquire physical insight.

Without accurate U-6Nb properties, the only meaningful validation is to verify that ABAQUS/Standard can accommodate problem-specific material properties and thermal boundary conditions. Based on prior experience it was established that, in general, anisotropic properties and time- and temperature-dependent heat generation can be accurately modeled. A determination as to how fine anisotropy can be discretized will have to wait until a typical microstructure has been calculated. To determine the code's ability to

define time- and position-dependent heat-transfer coefficients, a sample calculation was conducted using an artificial geometry. Nominal boiling coefficients were defined for five orientations: horizontal downward facing, slanted downward facing, vertical, horizontal upward facing, and slanted upward facing. A time dependence was calculated using immersion velocities typical of production facilities and superimposed on the coefficients. These data were input to ABAQUS/Standard, and the complete model was executed. It was concluded that results were real and that ABAQUS/Standard was capable of modeling problem-specific thermal boundary conditions.

Parametric studies will be conducted using the validated code and experimentally derived quench coefficients. A geometry model will be defined using typical prequench dimensional data and a series of runs made to identify material properties that have a significant effect on calculated distortion and residual stresses. These cumulative results will help establish the scope of additional studies to accurately define material properties and part distortion.

Casting Experimental Studies and Model Development

Predicting melt solidification, microstructure, and carbide flotation requires solving four coupled non-linear problems: (1) a *computational fluid dynamics* (CFD) calculation to define pouring, carbide flotation, and solidification; (2) a *computational heat-conduction* (CHC) calculation to define the transport of thermal energy through the mold; (3) an *electromagnetics* calculation to define induction-heater effects on mold temperatures and fluid convective currents; and (4) a *metallurgical* calculation to define microstructure. Because of the complexity of these coupled physics, each element will initially be studied separately. The CHC facet was addressed first because of its importance to the overall solution [Taylor and Mackiewicz-Ludtka, 1992]. This current effort defined the remaining problem elements and their related numerical issues.

Specific casting mechanisms to be studied using the laboratory-scale induction furnaces in the Y-12 Development Foundry include the following:

1. the effect of alloying agents, melt superheats, and part thickness on microstructure, carbide formation, and carbide flotation in the crucible and mold;
2. induction heating in the mold and crucible during heat-up;
3. heat conduction in the mold and crucible during heat-up, pour, and solidification;
4. thermal resistances, especially the melt/mold coefficient, during and after solidification; and
5. the effect of heating-coil magnetic field on flotation and solidification.

Specific modeling topics to be studied will include the following:

1. The rigor of commercial casting simulation software. Unlike the quench, where ABAQUS/Standard is considered globally adequate, there is some concern that currently available software will be unable to accurately model U-6Nb microstructure.
2. The use of tetrahedron rather than hexahedron finite elements. Although tetrahedrons are generally not desirable for CFD calculations because of their tendency for numerical dispersion, they do permit the use of auto-meshing software. This, in turn, reduces the cost of preparing analysis models.
3. The level of geometry approximation; that is, whether reduced-order approximations such as RZ axisymmetric will be adequate to achieve experimental agreement.
4. Maximum permissible solution time step. Small steps give more accurate results but cause increased execution times. Preliminary indications are that relatively small steps are required to model uranium in general and obtain stable flotation results. Accordingly, a systematic evaluation of this parameter is prudent.
5. The influence of the air region component of the induction-heating model on the accuracy of calculated mold temperatures.

6. The validity of assuming (1) that carbides are formed in the crucible prior to the pour and (2) that their final distribution in the part can be predicted by assuming that they behave as buoyant particles influenced only by fluid-particle density differences and fluid convective currents.

Casting System Description

Laboratory-scale casting studies will be conducted using a vacuum-induction casting system consisting of a casting assembly, a water-cooled induction heater, and a vacuum caster. The casting assembly has five components: a crucible, an upper-end cap, mold halves, and a lower-end cap. The standard geometry used for development studies is a rectangular bookmold and is shown in Fig. 7. All components are fabricated from ATJ-grade graphite, and surfaces that might come in contact with liquid uranium are coated with yttrium oxide. In addition, some number of platinum - 90% platinum / 10% rhodium thermocouples with aluminum oxide (Al_2O_3) insulating sheaths are installed in the crucible and mold. The induction heater is a 15-kW 10,000-Hz unit. The coil is permanently mounted in the vacuum caster and is formed from twelve turns of a single small-diameter copper tube. The vacuum caster consists of a pressure vessel, two vacuum pumping systems, and associated piping and valves. The pressure vessel is cylindrical and has a height and ID of approximately 110 cm. It is divided into two sections, a fixed bottom half and a hinged top to facilitate loading and unloading of the casting assembly.

Fig. 7. Unassembled bookmold casting-system components showing yttrium oxide coatings; from left to right, end caps, mold halves, and crucible.

When installed in the caster, the casting assembly rests on a firebrick base whose thickness has been adjusted to provide the desired casting-assembly/induction-heater alignment. The assembly is mechanically, electrically, and thermally insulated from the heating coil by a ceramic shield constructed from 96% pure Al_2O_3 . The shield is vertically positioned using small pieces of firebrick such that it is aligned with the top of the crucible. Melt temperature in the crucible is measured using a single platinum - 90% platinum / 10% rhodium thermocouple that has been placed in an Al_2O_3 thermowell. This configuration is shown in Fig. 8.

Casting Experiment Designs

Three casting systems were defined to characterize individual NNSC/WR physics. Their mechanical design, research goals, and execution sequence are discussed below.

Uranium and U-6Nb in a Crucible. This study will define quiescent (i.e., no-pour) solidification in a cylindrical crucible similar to the one shown in Fig. 7. The goal is to define unobstructed flotation and microstructure for bulky sections. The study will be conducted in two iterations. The first will evaluate the effects of different alloying agents and melt superheats on flotation using uranium. Table 3 summarizes the candidate agents. Hafnium has been previously studied [Mackiewicz-Ludtka and Taylor, 1991], and

zirconium (Zr) will be the first agent evaluated in this current effort. The second iteration will repeat the evaluations using U-6Nb. Transient-melt and crucible-wall temperatures from each run will be recorded for use with the numerical models. In addition, each solidified melt will be examined to define grain structure and inclusion distribution. These results will also be used to validate model predictions and make comparisons with obstructed-flotation results to determine the relative merit of quiescent solidification as a carbon-removal mechanism.

Fig. 8. Schematic illustration of vacuum-induction casting system showing assembled bookmold casting system.

Table 3. Candidate Carbon-Alloying Agents and Selected Physical Properties

Alloying Agent and Carbide Formed	Melting Point (K)	Standard Free Energy of Formation (kcal/mole)	Density (g/cm ³)
Niobium/NbC	3773	-32.2	7.82
Tantalum/TaC	4153	-34.1	14.39
Titanium/TiC	3257	-39.1	4.93
Zirconium/ZrC	3530	-44.2	6.73
Hafnium/HfC	4163	-50.9	12.97

U-6Nb in a Vertical Channel. These studies will be conducted using the bookmold geometry shown in Fig. 7. The goal is to define unobstructed flotation and microstructure in less-bulky U-6Nb parts for different alloying agents and melt superheats. Runs will be conducted in two phases. The first will utilize the induction heater just to melt the charge, and the second will extend the operation of the heater into the solidification period to determine the effect of magnetic fields on microstructure and carbide flotation. The first run of each phase will use the most effective alloying agent identified from the crucible studies. As before, melts will be examined to define metallurgical properties, and these results together with temperature data will be used to benchmark the numerical codes and assess the relative merit of quiescent solidification as a carbon-removal mechanism.

U-6Nb in a Slanted Channel. These studies will be conducted using the bookmold casting system modified to contain a narrow upward-sloping rectangular channel. This geometry, shown schematically in Fig. 9,

will simulate the mold cavities of some parts. The goal is to define obstructed carbide flotation and microstructure for narrow sections. As in the vertical-channel tests, separate runs will be made to determine the influence of alloying agents, melt superheat, and the continued operation of the induction heater. Again, cumulative data will be used to benchmark numerical calculations and assess the relative merit of quiescent solidification as a carbon-removal mechanism.

Construction of Casting Models

The ProCAST commercial casting code [UES, 1996] will be used to conduct casting analysis because it has the versatility to model the NNSC/WR physics being studied. The P3/PATRAN code [MacNeal-Schwindler, 1996] will be used to construct and mesh geometry models. This selection was based on its abilities to construct complex three-dimensional (3-D) models, manually mesh with hexahedrons, and automesh with tetrahedrons. Three models were constructed using this software, one for each experimental casting system described above. Their design reflects the dual requirement to provide a numerical tool to support the acquisition of physical insight and a computational testbed for systematically acquiring numerical insight into NNSC/WR physics. The overall execution sequence reflects the need to first define NNSC/WR mechanisms in order to validate the models and then to use them to acquire physical insight.

Uranium and U-6Nb in a Crucible. This model is a transient 3-D half-symmetric representation of the crucible and is shown in Fig. 10. The goal is to accurately simulate solidification, microstructure, and carbide flotation [i.e., the metallurgical figures-of-merit (MFOM)] during an unobstructed bulky-section quiescent solidification.

For model validation, initial melt temperatures and transient specified-temperature boundary conditions will be taken from experimental data. This will remove numerical uncertainties that would otherwise accrue from using calculated values. Parametric studies will then be conducted to define those numerical-solution parameters (e.g., time step) that provide the best experimental agreement. Following that exercise, the sensitivity of model predictions to material properties and the melt/mold heat-transfer coefficient will be studied to establish the need for follow-on studies to define accurate values. Initial values for the coefficient will be calculated using crucible transient temperature data and the localized inverse-heat-conduction data-reduction program used to reduce quench data.

Using the validated model, a range of arbitrary melt temperatures and specified-temperature boundary conditions will be studied to define the sensitivity of the MFOM in bulky parts to properties and the melt/mold interface heat flux.

Fig. 9. Inclined narrow-channel geometry.

Fig. 10. Three-dimensional crucible geometry model discretized using hexahedron finite elements.

The first iteration of the above sequence will use uranium rather than U-6Nb. This will remove uncertainties that would otherwise accrue from the underdefined U-6Nb properties. Additional iterations will be completed for different alloying agents, and then for U-6Nb and different agents. These cumulative results will help establish the need for accurate U-6Nb properties data. All of the above iterations will be conducted using a geometry model that has been discretized with hexahedron finite elements. To determine the acceptability of less rigorous discretizations, an arbitrary set of process conditions will be input to three less-precise models. These are 3-D half-symmetric with less-refined hexahedrons, 3-D half-symmetric with less-refined tetrahedrons, and an RZ axisymmetric with refined hexahedrons.

U-6Nb in a Vertical Channel: This model is an RZ axisymmetric representation of the bookmold casting system described above; that is, crucible and top, end caps, mold, firebrick base, insulating shield, and heating coils. Additionally, an air region is included for the induction-heating calculations. The complete casting system geometry and part of the air region is shown in Fig. 11. The goal is to accurately simulate the MFOM during an unobstructed postpour solidification of a less-bulky part.

Fig. 11. Axisymmetric (RZ) bookmold geometry model discretized using hexahedron finite elements.

Model validation will consist of quantifying heat transfer from exterior mold and crucible surfaces, establishing the accuracy of induction-heating calculations, and defining melt/mold heat-transfer coefficients for the vertical mold-cavity.

1. A steady-state version of the model with no uranium in the crucible will be executed to define heat-transfer from exterior surfaces. Heat conduction in the bookmold system has been studied previously [Taylor and Mackiewicz-Ludtka, 1992]. Also, accurate properties data exists for graphite, and ProCAST has excellent capabilities for calculating radiation heat transfer. Accordingly, the only uncertain conduction mechanism in an empty casting assembly is heat transfer from exterior surfaces. Two specific environments will be studied: conduction in the crucible-wall/insulating-shield/heater-

- coil area and radiation heat transfer across the void formed by the lower portion of the shield and the casting assembly. These localized geometry regions are also shown in Fig. 11.
2. Once these mechanisms have been defined, the steady-state model will be executed for a range of coil currents to establish ProCAST's accuracy for calculating initial mold temperatures. Ideally, this will show that actual current calculates actual temperatures. Alternatively, a correlation between actual and model-input current will be defined such that known temperature distributions can be duplicated. Initially, this analysis will use a geometry model with a nominal air-region. A second series of runs will be conducted using a more expansive region to define the model's sensitivity to this approximation.
 3. Time- and position-dependent melt/mold interface heat-transfer coefficients will be defined using experimental temperature data and the localized inverse-heat-conduction program.

Parametric studies will be conducted using the validated model to define the MFOM for a range of melt superheats, alloying agents, U-6Nb property values, melt/mold coefficients, and heater operation. In addition to quantifying NNSC/WR physics, cumulative results will help establish the need for individual studies to define properties and/or heat-transfer coefficients and to assess the relative merit of quiescent solidification as a carbon-removal mechanism.

U-6Nb in a Slanted Channel. This model, shown in Fig. 12, is a transient 3-D half-symmetric representation of the complete slanted-channel casting system. The goal is to accurately simulate MFOM during an obstructed post-pour solidification. Model validation will begin by determining the time- and position-dependent melt/mold interface heat-transfer coefficients for the slanted mold-cavity walls. These results will be input to the 3-D model together with previous vertical-channel results, and the resulting mold/crucible temperature distributions compared to experimental values. Ideally, the crucible and axisymmetric results will give acceptable agreement in the 3-D model. Alternatively, values will be redefined to maximize experimental agreement. Parametric studies will be conducted using the validated model to define MFOM for a range of melt superheats, alloying agents, U-6Nb property values, melt/mold coefficients, and heater operation. These cumulative results will be used to quantify NNSC/WR physics, to establish the need for rigorous geometry models and/or follow-on studies, and to assess the merit of quiescent solidification as a carbon-removal mechanism.

SUMMARY

The effort to develop the NNSC/WR process is well under way. Materials characterization studies of cast U-6Nb are complete. Preliminary results suggest that if the number and distribution of inclusions can be controlled, it should be possible to produce acceptable cast parts using significant

Fig. 12. Three-dimensional inclined-channel geometry model discretized using hexahedron and tetrahedron finite elements.

amounts of recycled material. Experimental studies to characterize casting and quench physics have been defined and are being implemented. Numerical models have been constructed using commercial software and are being informally executed to establish their readiness for use in the integrated experimental-numerical studies.

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