DEVELOPMENT OF AN ANALYTICAL MODEL PREDICTING MICROSTRUCTURE AND PROPERTIES RESULTING FROM THE THERMAL PROCESSING OF A WROUGHT POWDER NICKEL-BASE SUPERALLOY COMPONENT

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Abstract

An analytical process model was developed to predict the cooling γ' size resulting from the thermal processing of the wrought powder nickel-base alloy, MERL76. The approach taken was to define the isothermal γ' coarsening law and then treat continuous cooling processes as a series of short isotherms and incrementally calculate cooling γ' growth. Predicted γ' sizes correlated well with measured values. The γ' size prediction model was combined with a strength prediction equation and estimates made for strength in full-scale components. Predicted strength values also correlated well with measured values, demonstrating the utility of process modeling in optimizing processing of full-scale components.

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Background

As a technology, nickel-base superalloys are reaching maturity with the era of breakthroughs in alloy composition ending and the greatest potential benefits being in process optimization and control (Ref. 1). Over the years, researchers have studied and documented the role of alloying elements in the microstructural development and mechanical behavior of superalloys (Refs. 2 through 5) and have also characterized the relationship between microstructure and properties such as strength and stress rupture (Ref. 2). Additional work has shown that properties can also be improved by thermal mechanical processes such as direct aging (Ref. 6). In summary, nickel-base superalloys are strengthened via three primary mechanisms: solid solution (matrix) strengthening by elements like Cr, Mo and W; via grain size effects according to a Hall-Petch relationship; and via age hardening by precipitation of γ'. It is the unique strengthening behavior of the γ' phase that provides superalloys with the high temperature properties required to operate successfully in the demanding environment of gas turbine engines. Key characteristics of the γ' phase that influence its strengthening potential include its volume fraction, size and antiphase boundary energy. Because of the significant effect of γ' on the properties of nickel-base superalloys, a substantial effort has been expended in understanding the formation, nucleation and growth of the phase as affected by alloying and thermal processing, such as heat treat temperature and cooling rate (Refs. 3, 7 and 8).

In spite of the wealth of knowledge that exists, one of the most frustrating, time consuming and critical challenges facing superalloy metallurgists is the transition from sub-scale laboratory development to full-scale production. Properties measured full-scale are often inferior to those determined sub-scale due in part to differences in the cooling rate between the smaller sub-scale specimens and larger full-scale components. Historically, the transition from laboratory to production often resulted in significant development effort with full-scale material to restore the properties back to laboratory scale levels. To be successful in the coming era, this type of sequential (laboratory → production) alloy/process development is no longer acceptable. Concurrent engineering and computer-assisted process development will be trademarks of successful programs. Success has been demonstrated in relating analytically determined cooling rates in superalloy components to measured properties via empirically derived relationships between cooling rate and mechanical behavior (Ref. 9). Recently, more fundamental models predicting microstructure and strength based on theoretical principles have been developed for age hardenable aluminum alloys (Refs. 10 through 12).

This paper describes the development of an analytical process model predicting the microstructure resulting from the thermal processing of a wrought superalloy component. The microstructural model is combined with a strength prediction model currently under development at Pratt & Whitney which demonstrates the utility of applying the model to optimize thermal processing and component heat treat geometry.

The strategy used in developing the model was:

- Define the isothermal γ' coarsening law for the alloy
- Model the quench process as a series of isotherms and incrementally calculate the γ' growth

- Input predicted γ' sizes, measured grain sizes and volume fraction γ' and known composition into a strength regression equation and estimate strength

- Compare strength predictions to components with known properties.

Procedure and Results

Determination of the Isothermal Coarsening Law

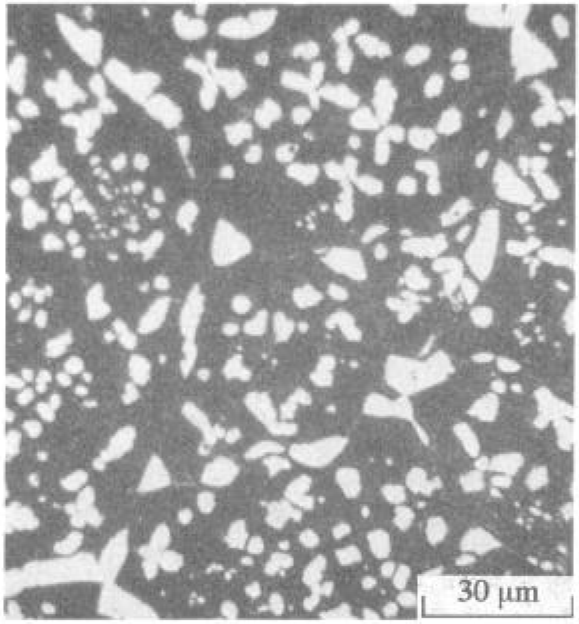
The isothermal γ' coarsening law is of the following form:

$$(\bar{r}^3-\overline{ro}^3)^{1/3} = A * (Ce/T)^{1/3} * t^{1/3} * \exp(-Q/3RT) \quad (1)$$

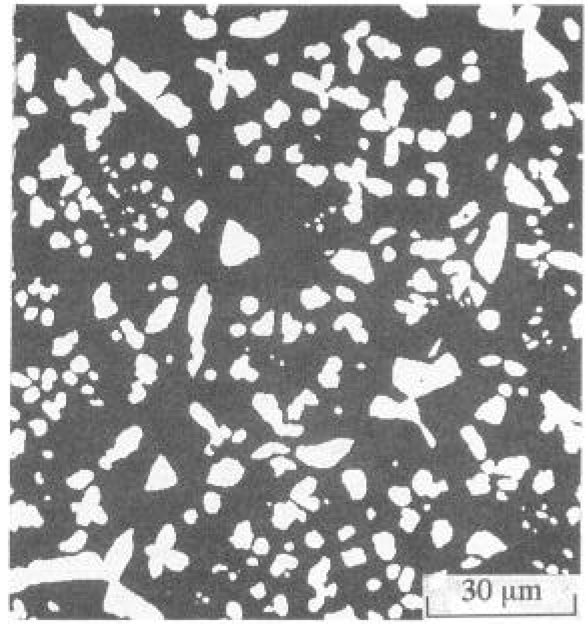
where:
- r = final γ' size in Å
- ro = initial γ' size in Å
- A = material constant
- Ce = equilibrium concentration (atomic percent) of Al and Ti in matrix at temperature T
- T = coarsening temperature in degrees K
- t = time in hours
- Q = activation energy for diffusion of Al plus Ti = 64500 kcal (Ref. 8)
- R = gas constant.

To define the coarsening law, it was necessary to determine a value for A and to define Ce as a function of temperature.

The alloy selected for this study was MERL76, one of the strongest alloys available commercially. It has been successfully fabricated via powder metallurgy techniques as a turbine disk material (Ref. 13). The nominal composition is presented in Table I. In order to establish Ce as a function of temperature, it was first necessary to determine the volume fraction γ' stable at various temperatures. This was accomplished by giving the material a supersolvus heat treatment (1204°C/2 hrs) to completely solution the γ', slow cooling (at rates of 1 to 3°C/hr) to the temperature of interest, followed by a rapid quench to room temperature. The slow cool precipitated the stable γ' as large particles. The γ' in solution at the temperature quenched from then precipitated as very fine particles. Samples were metallographically prepared and elecrolytically etched with a 30 percent Phosporic acid solution which attacked the γ matrix, leaving the γ' in relief. The region containing fine γ' exhibited a speckled appearance with the coarse γ' appearing as large, white particles. The structures were stored as digitized, grey level images and processed through a series of image enhancement routines using a Zeiss IBAS Image Analysis System which accentuated the contrast between the coarse γ' and the balance of the microstructure (Fig. 1). This allowed for easy measurement of the area percent coarse γ'. The area percent measurement was assumed to be equal to the volume percent. Consistent with a previous investigation (Ref. 8) of a high volume fraction γ' alloy, it was assumed that all the γ' had precipitated out by 871°C. The area percent γ' measurements are presented in Fig. 2. The total area percent γ' measured is consistent with previously reported volume fraction γ' for MERL76 (Ref. 14). By knowing the volume fraction γ' stable as a function of temperature, assuming the composition of the γ' remains constant (Ref. 8) and calculating the composition of the γ' in MERL76 (Ref. 14), the amount of Al and Ti in the matrix can be determined as a function of temperature through use of a modified lever rule for a pseudo phase diagram. The relationship between Ce and temperature for MERL76 is presented in Fig. 3 and can be approximated by a linear relationship at temperatures above 871°C. At temperatures of 871°C and below, Ce = 5.6 which is the calculated amount of Al and Ti in the γ matrix.



(a) As Etched



(b) Digitally Enhanced

Fig. 1 Slow Cooled Specimen Showing Stable γ′ as Coarse Precipitates

Table I. Nominal Composition of MERL76 (Weight Percent)

Al	Ti	Nb	Co	Cr	Mo	Hf	C	Ni
5	4	1.5	18.5	12	3	0.5	0.02	Bal.

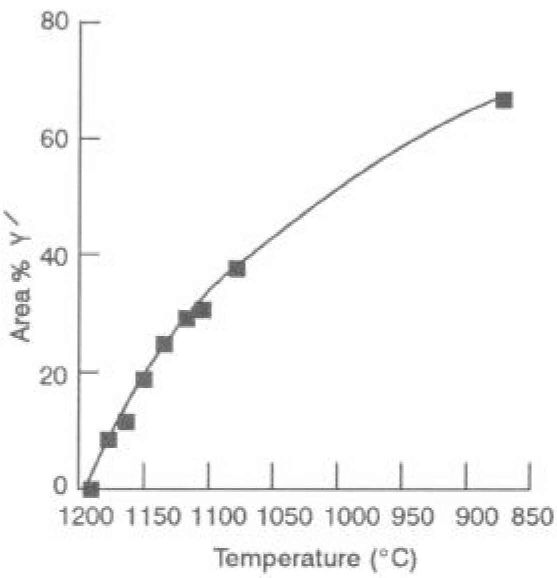


Fig. 2 Area Percent γ′ Stable at Various Temperatures for MERL76

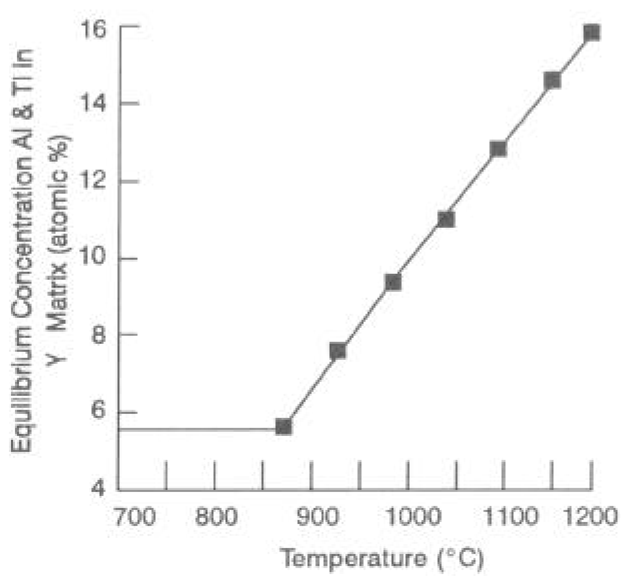


Fig. 3 Equilibrium Matrix Concentration of Al and Ti (atomic %) as a Function of Temperature for MERL76

To determine the value of the constant A, a total of 12 isothermal heat treatments were conducted over the temperature range of 816°C to 982°C for times of 0.5 to 24 hours. The γ' size was measured via TEM replication both before and after heat treatment. The results are presented in Table II. For each of the isothermal heat treatments, a value for A was determined by solving the coarsening equation and the values are listed in Table II. An average was determined ($A=1.91 \times 10^7$) and used for the coarsening equation. Predictions were made for the isothermal heat treatments and are listed in Table II and compared with measured values in Fig. 4. In general, the coarsening equation overpredicts γ' growth at finer starting sizes and underestimates growth at coarser starting sizes.

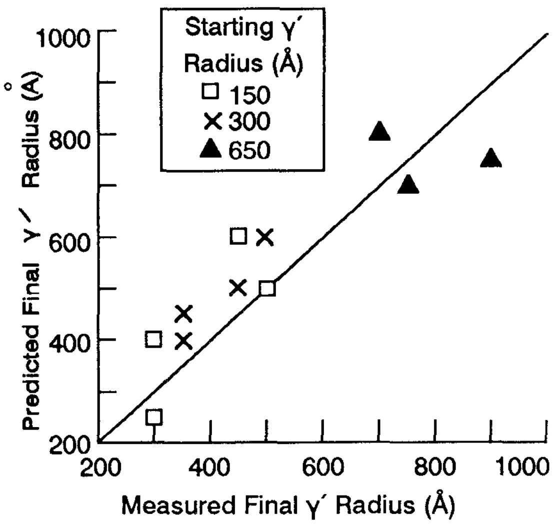


Fig. 4 Comparison Between Predicted and Measured γ' Sizes After Isothermal Heat Treatments for MERL76

Table II. Measured and Calculated Cooling γ' Growth After Isothermal Exposures

		Measured γ' Radius		Calculated	
Temperature (°C)	Time (hrs)	Initial	Final	Final Radius	A (x 10^7)
816	8	300	350	400	1.415
816	8	650	750	700	2.975
816	24	150	500	500	1.935
816	24	300	450	500	1.565
816	24	650	900	750	3.000
871	0.5	150	300	250	2.565
871	3	150	300	400	1.410
871	3	300	350	450	1.235
871	3	650	750	700	2.635
982	1	150	450	600	1.415
982	1	300	500	600	1.470
982	1	650	700	800	1.305

Application of the Isothermal Law to Continuous Cooling

The initial attempt to model the microstructural evolution during continuous cooling was made using instrumented cubes approximately 7.6 cm on edge. The cubes weighed about 4 kg and were instrumented with 3 thermocouples (T/C) at depths of 0.6, 1.3 and 3.2 cm. The cubes were solutioned at 1079°C and air, forced air, water or oil quenched. Temperatures were recorded in 1 second intervals. The γ' size was measured at the base of each T/C location and the results are presented in Fig. 5a (air cool) and Fig. 5b (oil quench). The approach taken to predict as quenched γ' size was:

1. Initialize starting γ' size (assume nuclei of 200Å) and time interval for cooling
2. Use time interval to measure temperature drop and calculate average temperature
3. Use average temperature to calculate Ce and incremental γ' growth
4. Use calculated incremental γ' size as the initial γ' size for the next time interval.

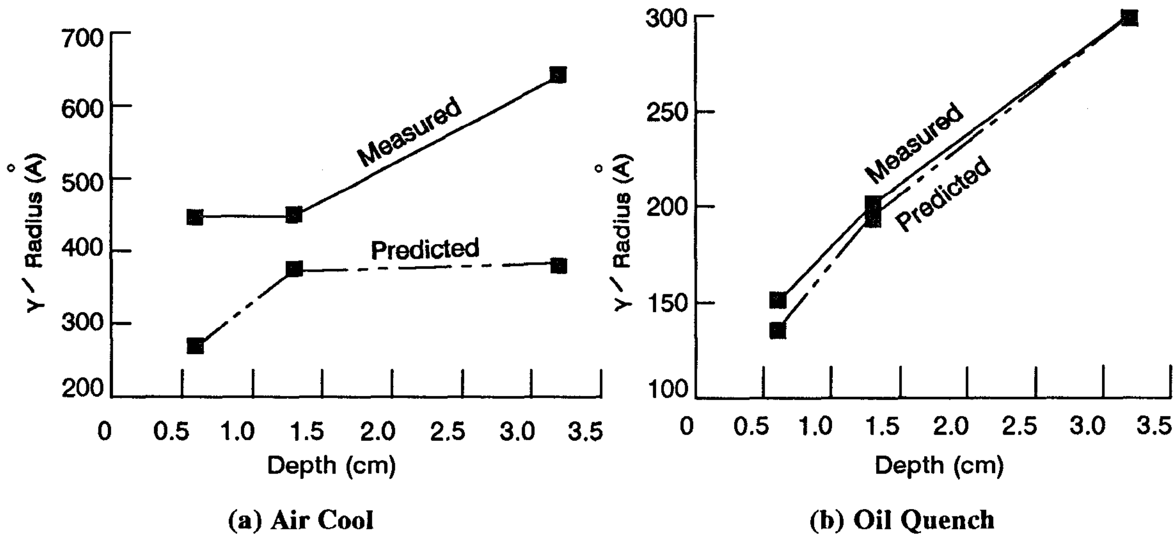


Fig. 5 Predicted Versus Measured γ' Sizes for Cubes Cooled At Various Rates from 1079°C

Predicted γ' sizes are compared with measured sizes in Fig. 5. Correlation is good for the faster cooling rates (oil quench) and poor for the slower cooling rates (air cool). The reason for the inaccuracy of the model at slow cooling rates is not fully defined. Initial work (Ref. 15) suggests that a growth process other than diffusion controlled coarsening is contributing. Sensitivity calculations (Ref. 15) showed the predicted γ' size was not significantly affected for assumed nuclei of 10 to 200Å or if the thermal step was kept to less than 66°C. Because of the success of the model in predicting γ' size after rapid quenches which is relevant to processing of production components, the strategy was applied to a full-scale disk.

A V2500 high-pressure turbine disk (weighing approximately 140 kg) was selected as the test vehicle. A finite element model was created and a disk instrumented with 17 surface and 3 imbedded T/C's (Fig. 6). The disk was oil quenched from 1079°C and temperature data collected electronically at a rate of approximately 20 readings per second (1 reading per T/C for each second of the quench). Heat transfer coefficients were back calculated from the measured temperatures for the disk configuration. The heat transfer coefficients were then used to predict the temperature distribution throughout the disk. An approach similar to that used for the cubes was applied to the disk with the following exceptions:

- Starting γ' size set at 10Å (more realistic estimate of nuclei size)
- Thermal step held constant at 14°C
- Heat transfer model used to determine time increment for 14°C thermal step.

Predictions for as quenched γ' size ranged from 230 to 380Å (Fig. 7). Measured γ' sizes ranged from 300 to 500Å and correlated well with the predicted values for the faster cooling near surface regions. Similar to the cube results, the γ' size was underpredicted for the slower cooling, thick sections of the disk (Fig. 7).

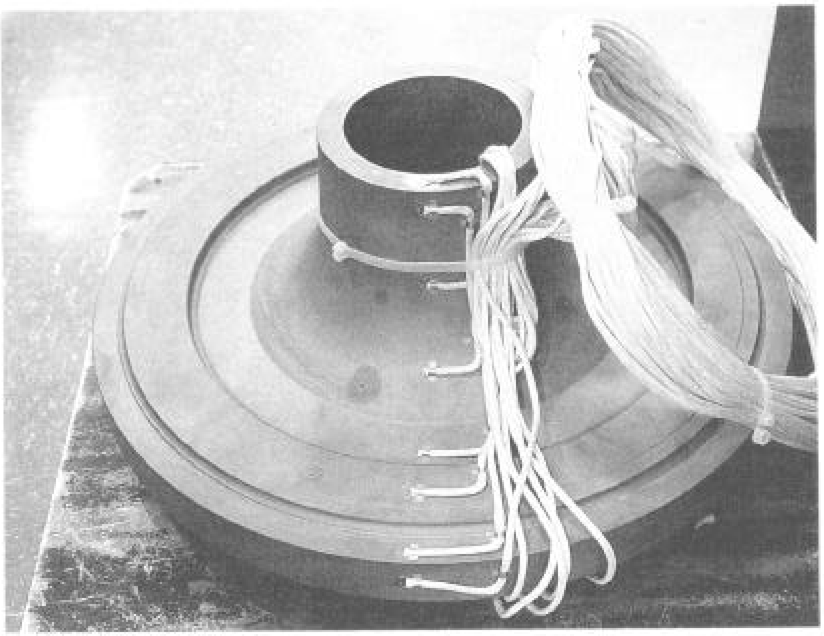


Fig. 6 Instrumented V2500 High Pressure Turbine Disk Used to Establish Heat Transfer Model

The microstructural prediction model was combined with a strength prediction model for nickel-base superalloys now under development at Pratt & Whitney. The strength prediction model is based on regression analysis of tensile specimens from wrought alloys of known composition and detailed microstructural characterization. There are 23 alloy compositions included in the regression. The correlation plot for the strength prediction model is presented in Fig. 8. The regression equation takes the form of:

$$482°C\ \sigma_{Yield}\ (MPa) = x_1 + x_2\,(Comp) + x_3\,(\gamma'_{VF})^{1/2} + x_4\,(Grain\ Dia.)^{-1/2} - x_5\,(\gamma'_{size})^{1/2} \tag{2}$$

where: x_1 to x_5 = equation constants
Comp = alloy composition in atomic percent
γ'_{VF} = volume fraction cooling γ'
Grain Dia. = average grain diameter
γ'_{size} = cooling γ' size.

The composition of the instrumented disk was known, volume fraction determined using Fig. 2 and grain size measured. These were input into the strength equation together with the predicted γ' sizes and estimates for 482°C yield strength determined. Predicted strength values ranged from 1041 to 1060 MPa which agreed well with test data on specimens machined from the disk (Fig. 9). Measured strengths ranged from 1054 to 1061 MPa.

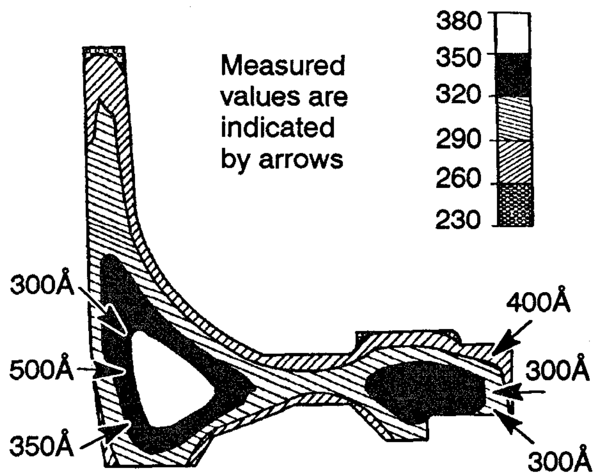


Fig. 7 Predicted Versus Measured γ′ Size MERL76 Disk Forging Quenched from 1079°C

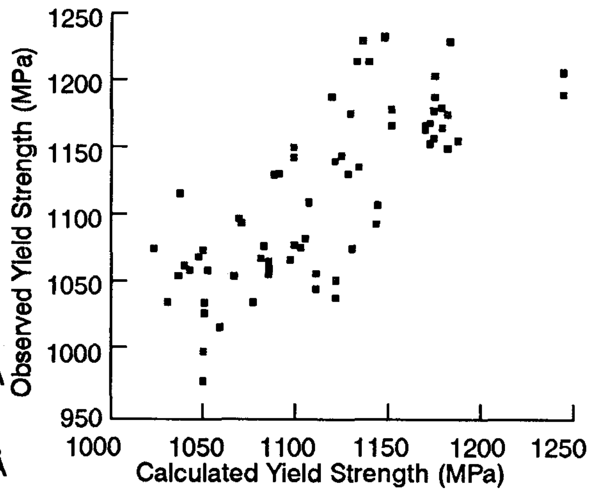


Fig. 8 Measured 482°C Yield Strength Versus Predicted for Tensile Regression Model

Applications of the Combined Strength/Microstructure Model

To demonstrate the utility of the combined microstructure/strength model, the strength of a similar disk geometry processed through a different heat treatment was predicted. Because the compositional contribution to strength (from the model) is independent of solution temperature, the only variables affected are microstructural. Fig. 2 shows the volume fraction cooling γ′ as a function of temperature; γ′ size is predicted by the thermal model leaving the effect of solution temperature on grain size unknown. When this was determined (Fig. 10), the contribution of the different microstructural features as a function of solution temperature (Fig. 11) was calculated for surface and center sections of the disk (only cooling γ′ size is affected by section thickness). The individual contributions were added together and combined with the compositional effect. The predicted strength levels (Fig. 12) were compared with strengths measured on test specimens machined from a disk given the thermal cycle, and excellent agreement was observed (1145 MPa predicted versus 1117 MPa measured).

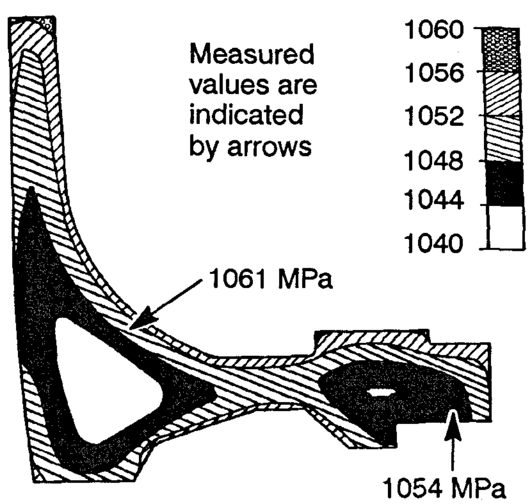


Fig. 9 Predicted Versus Measured Yield Strength MERL76 Disk Forging Quenched from 1079°C

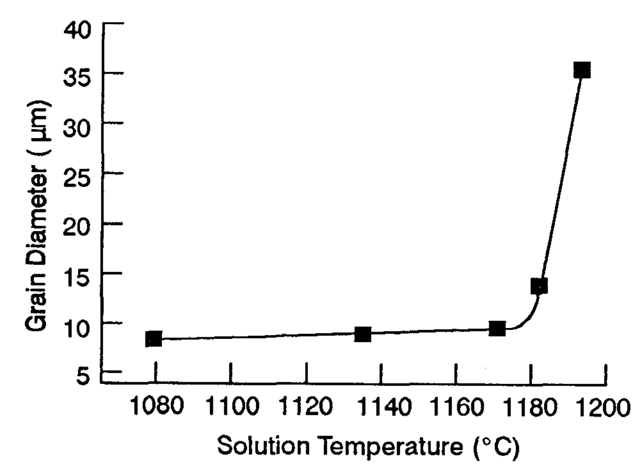


Fig. 10 Effect of Solution Temperature on the Average Grain Diameter of MERL76

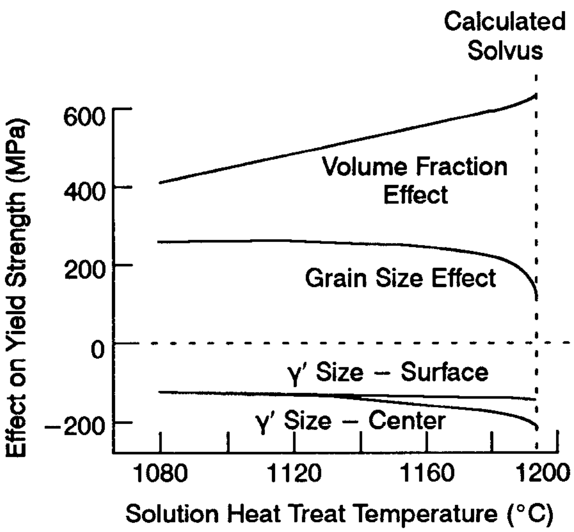


Fig. 11 Calculated Microstructural Effects on 482°C Yield Strength

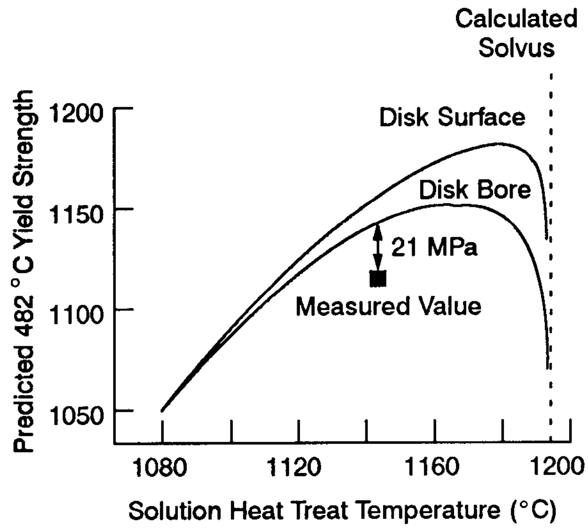


Fig. 12 Predicted 482°C Yield Strength for MERL76 at 1143°C. Measured value is 21 MPa below predicted.

Summary

An analytical model was developed by applying the isothermal γ′ coarsening law to a continuous cooling situation to predict the microstructure in full-scale components. The microstructural model was combined with a strength prediction equation, and good correlation was observed between predicted and measured strength values.

The combined microstructural/strength prediction model shows the potential benefits associated with analytical process modeling. For a given alloy composition, both the thermal processing and component heat treat configuration can be optimized prior to processing of an actual part. The potential exists to take into consideration the property gradients that exist in the part during design. The challenges for the future are to:

- Develop models to predict grain size, volume fraction γ′ and γ′ coarsening as a function of composition

- Broaden the model to include other mechanical properties.

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