The Application of CALPHAD Techniques in the Development of a New Gas-Turbine Disk Alloy

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Introduction

The development of a new nickel-based superalloy for use in the high-pressure turbine disk of a modern gas turbine is one of the most expensive and protracted exercises undertaken by gas-turbine manufacturers. A typical complete development cycle can take more than 10 years. This delay arises not only because of the extensive mechanical testing and validation required to ensure the safety of the critical part, but also because of the difficulty of finding a material chemistry that provides the correct degree of balance between mechanical properties and long-term material stability. The conventional approach to this latter problem is to use a combination of experience, empirical wisdom, and a few basic calculation tools based on electron-valency theory (PHACOMP).[1] There is thus an urgent need to develop a tool that reliably summarizes the known body of knowledge about the stability of Ni-based superalloys and provides a method that can quickly and reliably guide the alloy developer through the initial alloy-chemistry selection phase of development.

Calculation of phase equilibria using calculated phase-diagram (CALPHAD) techniques[2] has now matured to the point where it is possible for the alloy developer to quickly and reliably calculate phase equilibrium in a matter of minutes without an in-depth knowledge of thermodynamics. There thus exists a tool that enables the definition of alloy chemistries so that specific assumptions can be tested and the final chemistry selected without having to carry out the traditional manufacturing, processing, testing, and examination of a large raft of experimental chemistries. This article aims to show how such a tool has been used and highlights the success of this approach in the field of Ni-based superalloy development.

Background

The gas turbine has its origins in the pioneering work of Sir Frank Whittle in the late 1930s. The world's first practical jet engine, the Whittle W1, flew in the Gloster E28/39 on May 14, 1941. This engine weighed approximately 1,200 lbs and developed about 860 lbs of thrust. The engine was primarily made of chromium steel, and the peak gas temperature was about 600°C. The modern successor to this engine in civil applications is the high-bypass turbofan, which powers aircraft such as the Boeing 777 and the Airbus 330. Typical of this type of engine is the Rolls-Royce Trent family of engines (Figure 1), which typically weigh 16,000 lbs (7.5 tons) and can produce in excess of 110,000 lbs of thrust. Gas temperatures in these engines are in excess of 1200°C. To achieve the equivalent thrust, one Trent would have to be replaced by 127 Whittle W1s. Conversely, to equal the power-to-weight ratio of the Whittle W1, the Trent would have to

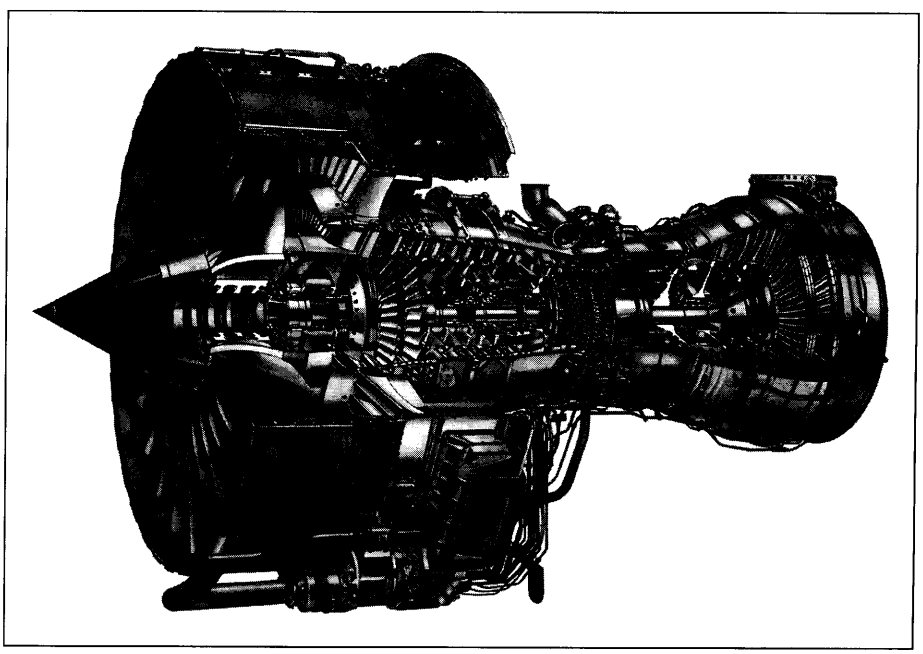

Figure 1. General-arrangement drawing of a Rolls-Royce Trent engine.

weigh 68 tons. These increases in performance have been achieved through improvements not only in engineering and aerodynamics but also in materials and the conditions that they can tolerate without catastrophic, rapid degradation or failure. One of the best examples of such materials are Ni-based superalloys that are used to make the high-pressure turbine disk. In this application, these alloys (Table I) operate at a peak metal temperature of 660°C and rotate in excess of 10,000 rpm. The component is thus very heavily loaded and exposed to very high temperatures for a significant portion of its life, which may be 10,000 h or more. Furthermore, gas-turbine design engineers always seek to increase the operating temperature of the engine to improve its overall thermodynamic efficiency. This leads to a requirement for alloys with an ever-increasing temperature capability. Stability of the microstructure and good mechanical properties at high temperatures are thus essential, as failure of such a part cannot be contained, and damage to the aircraft on this scale may have catastrophic consequences.

The Ni-based superalloy most recently introduced for this application in Rolls-Royce gas turbines is the alloy 720Li (Table I). This material was derived from a turbine-blade alloy via a number of empirical modifications and is capable of operation at temperatures up to 650°C. Above this temperature, the alloy's properties degrade rapidly because of the precipitation of sigma phase. This phase originates in the Ni-Co-Cr-Mo-W system and is extremely brittle. It can grow in a blocky form along the grain boundaries, thus introducing the possibility of sudden, unexpected crack growth along these boundaries. It also causes Cr and other beneficial elements to be depleted in the material close to the grain boundary. Also, in comparison to another standard Ni-based superalloy used in this application, Waspaloy (Table I), 720Li has a significantly lower resistance to fatigue-crack propagation. Thus to meet the high-pressure turbine disk requirements of modern engines, a new Ni-based superalloy capable of overcoming these limitations and coping with higher temperatures was needed.

Initial Alloy Design

Based on the capabilities of Waspaloy and 720Li, and the requirements for future gas turbines, four alloy design targets were set:

(1) An ultimate temperature capability of 725°C.

(2) A fatigue-crack-propagation resistance equivalent to that of Waspaloy (roughly an order of magnitude better than that of 720Li).

(3) Better creep resistance than 720Li and Waspaloy.

(4) An ultimate tensile strength equivalent to 720Li.

At the time the alloy-development program was initiated, an appropriate CALPHAD model was not available, and therefore, a traditional alloy-development approach was adopted. A base-line chemistry was defined using information available in the open literature, the alloy developers' own experience of working with Ni-based superalloys, and a knowledge base of the modifications in chemistry that had improved alloys in the past. The initial phase of the program was to manufacture multiple variants of a base chemistry and test their mechanical properties. The overriding concern at this stage was stability, so seven variants were chosen, using the PHACOMP approach.[1]

PHACOMP relies on the concept of an averaged electron-hole number, which is made up of the weighted average electron-hole numbers for the elements being considered. It is simple and quick to use and produces a number which can be used as a measure of the degree to which an alloy is prone to sigma-phase precipitation. The larger the number, the more sigma-prone the alloy is. Within a PHACOMP scenario, the concept of "sigma safe" means the average electron-hole number $\bar{N}_v$ of the alloy would be below a critical value, and the alloy will be sufficiently stable for practical application. However, this critical value is not necessarily a fixed number and may often be found by experience for each alloy. Due to its simple nature, the use of PHACOMP does not allow for the true complexity of topologically close-packed (TCP) phase formation to be taken into account, and other deleterious phases such as mu, P, R, and Laves are not considered. Furthermore, PHACOMP gives no information on temperature ranges of stability or phase boundaries. However, it was the only tool available at the time, and in the past, it has been a useful guide in the development of new alloys.

The seven variants were manufactured, tested, and examined. Based on a balance between the amount of sigma precipitation and the requisite achievement of mechanical properties, a base alloy was defined for further development.

Refining the Chemistry

Based on metallographic examination, the new alloy was considered to be sufficiently stable for practical applications, and its mechanical properties were near to the set targets. Twelve further variations of this "phase two" chemistry were then defined, based on making small variations near the base chemistry so that a judgment on alloying limits could be made (Table II). This is important for future manufacturing, because if the alloy becomes catastrophically unstable or fails to meet the required properties because of small changes in chemistry, then it may not be possible to manufacture it within normal composition tolerances. The alloy would thus be prohibitively expensive to manufacture because of the special melting requirements.

The new alloys were manufactured, tested, and examined, and a chemistry was defined that provided the desired properties with a very high degree of stability; this was considered to be the final development-alloy chemistry. At this point, it was decided to scale up the development program. Because of the number of variants in the system, manufacturing and testing until now had been limited to 1–2-kg bars. In the final phase, the process was scaled up to 50-kg melts. With material now available on a larger scale, trial turbine disks could be manufactured using forging conditions that were representative of final production-forging practice.

Based on the alloy as defined from phase two, and two slight variations as a "look-see" at a final modification to the chemistry, three alloys were produced for the scaled-up trials. All three alloys exhibited the desired excellent stability;

Table I: Alloy Chemistries of Superalloys Used in Rolls-Royce High-Pressure Turbine Disk Applications.

	Ni	Co	Cr	Mo	W	Ta	Ti	Al	B	C	Zr	Hf
720Li	Bal	14.75	16.00	3.00	1.25	0	5.00	2.50	0.015	0.025	0.035	0
Waspaloy	Bal	13.5	19.5	4.3	0	0	3.0	1.3	0.006	0.08	0.06	0

Table II: "Phase Two" Chemistry Variations of the Development Alloy.

Alloy Variant	Reason	Comments
Base alloy	Derived from initial experimental series	
2	High Al, low Ti	High gamma-prime content within normal alloy-melt chemistry tolerances.
3	Low Al, high Ti	Low volume fraction, high-strength gamma prime within normal alloy-melt chemistry tolerances.
6	High Mo	High solid-solution-strengthened matrix, lower stability with respect to mu-phase formation.
9	Low Mo	Low strength, high stability.
11	High Ta	High volume fraction, high-strength gamma prime.
13	Low Ta	Low volume fraction, low-strength gamma prime.
14	Inclusion of Hf	To gauge effectiveness of Hf addition, based on blade-alloy development experience.
16	Low Cr	High stability with respect to TCP (topologically close-packed phase) formation, lower oxidation resistance.
19	High Cr	Destabilized with respect to TCP formation, high oxidation resistance.
20	Low Co	To judge effects of Co.
21	High Co	To judge effects of Co.
22	Partial Re substitution for Mo	To assess effects of Re (read over from blade-alloy development).

only minor mu-phase precipitation was observed, and the alloys met most of their mechanical design-property targets. However, they did not meet one of the major alloy-design criteria, the crack-propagation-resistance requirements. We realized that our understanding of the alloy-chemistry effects was inadequate and that some of the empirical rules that had been followed were either wrong or did not go far enough. For example, the PHACOMP approach said that the alloy was sigma safe, but it was now precipitating mu phase. In this circumstance, what useful information did the PHACOMP calculation actually provide? A new approach to the problem had to be found that would enable the alloy-development program to recover.

Introduction of the Phase-Diagram Model

During the initial development phase of the alloy, it was recognized that the CALPHAD technique was sufficiently advanced to enable calculation of phase equilibria in real multicomponent systems. There was thus the possibility of producing accurate equilibrium predictions of phase amounts, phase chemistries, and the effects of chemistry variations. Also solidus, liquidus, and phase-transition temperatures could potentially be defined, opening up the possibility of testing the alloy for processability without having to actually melt a test sample.

Development of a suitable CALPHAD model to support future Rolls-Royce Ni-based superalloy development was therefore initiated. The model required that thermodynamic parameters for the multicomponent system Ni-Al-Co-Cr-Hf-Mo-Ta-Ti-W-Zr-B-C be produced, stored in a new database, and the resultant multicomponent calculations be validated against known behavior of real Ni-based superalloys. The construction of the new database has been described previously[3] and predicted results for features such as solidus, liquidus, gamma-prime solvus, and amount of gamma prime in an alloy. The composition of gamma and gamma prime was tested against values reported in the extensive literature. It was demonstrated that the error on phase-transition temperatures, phase chemistries, and phase amounts using the new CALPHAD database was close to that expected from carrying out experimental measurements.[2,3] This validation process was a critical part of the database development and, for the first time, allowed predictions for real Ni-based superalloys to be made with high levels of confidence. Effectively, the CALPHAD route was providing a rapid experimentation route that allowed critical features to be *quantitatively* defined and used in the alloy design process. The new database has been used with two software packages, MTDATA[4] and Thermo-Calc.[5] Furthermore, utilizing a new computer interface to Thermo-Calc called ETTAN, it was possible for nonspecialists in the field of phase diagrams to produce computed results that could be immediately understood and used on an everyday basis.

A New Direction

When the third series of alloys did not meet the crack-propagation-resistance target, it was thought that, although a series of very stable alloys had been developed, there may be a link between stability and mechanical properties which was not understood. It was also found that crack-propagation tests carried out in air failed to meet the target, while those carried out in vacuum met the target. This implied that oxygen ingress down the boundaries could be one of the controlling factors in crack propagation. It was also noted that the primary MC carbides were so stable that they were not breaking down in the expected way to $M_{23}C_6$-based carbides on the grain boundaries. Other Ni-based superalloys have some degree of precipitation on the grain boundaries, usually a combination of Cr- and Mo-based phases related to $Cr_{23}C_6$, M_6C, sigma, and mu. These factors suggested that the alloy stability needed to be modified in such a way that a Cr-rich phase, either sigma and/or one of the carbides, would be precipitated on the grain boundaries. Because the new CALPHAD model allowed specific features of phase equilibria to be calculated, it was used to design a series of alloys to specifically test this and other theories. Variations of the base alloy from the "phase three" work were run through

the model and modified until the desired phases, phase amounts, and heat-treatment windows were available to achieve the desired results (Table III). The test matrix was also reduced, as it was possible to design alloys with given properties while holding other variables constant; for example, alloys were designed to precipitate given amounts of sigma with a defined start temperature while holding the amount of gamma prime and gamma-prime solvus temperature constant. All of the alloys could thus be processed the same way, allowing processing variations to be removed as a variable in the test matrix.

By using this model, the program was able to complete the manufacture, test, and examination cycle within 15 months. During this work, it was also shown that although CALPHAD modeling produces predictions that strictly apply only to equilibrium conditions, the results can be applied to the real nonequilibrium case, provided that the kinetics are understood from practical experience. The alloy-development team found that they had more relevant information on the effects of chemistry on phase equilibria in such a complex system than they ever had before, that the information was readily accessible by nonspecialists, and that it could be generated in a very short time. The alloy-development experiment on the computer was deemed a success.

Table III: "Phase Three" Chemistry Variations of the Development Alloy.

Alloy Variant	Reason	Comments
Alloy A	Derived from "phase two" alloys	Originally thought to be the final alloy chemistry.
Alloy D	High Cr addition	Promoted instability and precipitated sigma on grain boundaries.
Alloy E	Rebalance Cr/Mo ratio to precipitate $M_{23}C_6$ on grain boundaries	Derived from alloy A.
Alloy F	Rebalance Cr/Mo ratio to precipitate M_6C on grain boundaries	Derived from alloy A.
Alloy G	High-Zr variant of alloy E	M_6C plus high Zr content on grain boundary.
Alloy H	High-Zr variant of alloy F	$M_{23}C_6$ plus high Zr content on grain boundary.
Alloy I	Re addition to alloy E	Mo reduced to compensate on sigma stability and keep carbide content constant.
Alloy J	Re addition to alloy F	Mo reduced to compensate on sigma stability and to keep carbide type and overall content constant.
Alloy K	Addition of Hf	Single addition based on blade technology additions.
Alloy L	Low-B variant of alloy E	Attempt to decrease and increase grain-boundary boride precipitation.
Alloy M	High-B variant of alloy E	
Alloy N	Variant on Ti/Al ratio	Change in gamma-prime volume fraction while keeping gamma-prime solvus temperature constant
Alloy O	Variant on Ti/Al ratio	
Alloy P	Variant on Ti/Al ratio	

Outcome

Based on the experimental data generated from the alloys designed with the phase-diagram model, valuable insight was gained into what was governing stability and crack propagation in the development alloy. The two major findings were

(1) stability with respect to sigma-phase formation is very sensitive to aluminum content because of the increased gamma-prime content and subsequent rejection of Cr and Mo into the surrounding gamma matrix, and

(2) a degree of instability is required in the alloy with respect to both carbides and sigma-phase formation, such that these phases could be precipitated at the grain boundaries in controlled amounts.

It was also found that the phase-diagram model allowed accurate judgment of the degree of instability to be made while controlling other variables. A final alloy chemistry could thus be defined, together with practical alloying limits also based on the model's predictions. This removed another risk from the alloy-development program and enabled a rapid manufacturing and testing cycle to be undertaken. The final alloy met all of its design targets.

Conclusions

The final design of the new Ni-based superalloy was a balancing act between stability and mechanical properties. The alloy could not have been designed within the time frame and cost of the overall program without using the CALPHAD model. There was no other way to carry out the sensitivity study required to judge where the balancing point was, without a prohibitively expensive and time-consuming trial program. The lessons that have been learned are

(1) the use of CALPHAD techniques to support the alloy design process is a real and practical possibility for industrially relevant alloys;

(2) the success of the technique depends critically on the use of a high-quality, *validated* thermodynamic database;

(3) with appropriate software, the CALPHAD model can be readily used and its output understood by nonspecialist phase-diagram modelers;

(4) the use of the model reduces the cost of the alloy-development program by reducing the risk that the alloys will not behave the way they were intended to and by shortening the alloy design process; and

(5) use of the model also expands the understanding of the underlying fundamental phase equilibria that govern how an alloy behaves. This allows carefully tailored alloys to be developed and opens up new avenues of alloy design.

Production of the new alloy is currently being scaled up and is due to find its first application in the Rolls-Royce Trent family of gas turbines just after the millennium.

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model in such an application could not have been demonstrated.

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