

# Accelerating Materials Research for indigenous Jet Engine Development: Integrated Computational Approaches

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## Abstract

The article presents the identified gaps(challenges) and their potential resolution methods pertaining to the development of an indigenous jet engine. It aims to accelerate the Kaveri program by implementing strategic projects to resolve the existing bottlenecks.

## 1 The Kaveri program

The GTRE GTX-35VS Kaveri is the Indian attempt at building an indigenous afterburning turbofan engine. The project is overseen by the Gas Turbine Research Establishment (GTRE) which is a lab under the Defence Research and Development Organisation (DRDO), Bangalore. The engine was originally intended to power the HAL Tejas Light Combat Aircraft (LCA) being builed by the Aeronautical Development Agency (ADA). But the Kaveri programme was delinked from the Tejas programme due to its failure to satisfy the necessary technical requirements. The GE-F404-IN20 engine is being used in LCA Tejas instead.

### 1.1 Challenges:

DRDO has not officially admitted any reasons or causes for the failure of the programme. From what has been reported in the media [8][12][17][23][22] following the delink, we come to the enlisted understanding of the shortcomings of the Kaveri programme.

- Performance: Decayed performance at high altitudes, insufficient thrust (52kN dry and 81kN afterburner) and noise at high throttle testing etc.
- Combustion: Combustion flicker, Lack of expertise in combustion research and flame control at high pressures etc.

- Materials: Thermal Barrier Coatings (TBC), High Temperature Ceramics, Directionally solidified and single-crystal turbine blades, Integrated blade and disk (BLISK) technology, Titanium alloys etc.
- Design: Unacceptable levels of fan-blade flutter risk, Reheat oscillations, First stage low-pressure compressor blade vibration etc.
- Aerodynamics: Lack of High End Computing Computational Fluid Dynamics tools and wind-tunnel test facilities in India. Kaveri failed its high altitude tests in Russia, 2004 at CIAM and 2010 at GFRI.
- Foreign collaboration: Disagreements between the French aerospace company, Safran and DRDO on cost terms for a joint development.
- Organisational structure, management and funding streams (2,133 crore) are all widely blamed by media.

It is apparent from the above points that the challenges are complex and interconnected. Any proposed resolution has to take into account this complexity and must be analysed for impacts on the whole system. But as each kind of gap requires a detailed survey and understanding of the subject

## 2 Literature survey

Information on the materials used in military jet engines is not available on the internet and therefore we must look into the materials used in commercial jet engines. It is important to note that due to different performance requirements of the commercial and military engine, the materials used in them differ, their processing methods differ and so does everything related.

The goal of the material selection process is to identify and manufacture materials that can withstand the high-temperature and high-stress environment inside the engine. On top of that they have to be corrosion, creep and fatigue resistant. The most critical component of the engine is its high pressure turbine blades. The material used in those blades is the single-crystal Ni-base superalloy.

### 2.1 Ni-base single crystal superalloys:

The turbine blades are made from Ni-base superalloys and are typically fabricated using Investment casting. They have one of the three kinds of microstructure, equiaxed or polycrystalline, directionally solidified and single crystal. The single crystal casting process, due to its complexity, has a significant cost associated with it. It is estimated that a set of 40 single crystal blades costs USD 600,000 (INR 4,50,19,800) [2]. Moreover the defects accumulated on them due to service cannot be restored with the current manufacturing methods.

#### 2.1.1 Material design:

Single crystal (SX) blades are produced via investment casting using high- $\gamma'$  nickel-base superalloys. Due to the intricacies of cooling channels in the blades, no machining process could be used to manufacture them.

Ni-base superalloys mainly comprise of intermetallic  $\gamma'$  precipitates in a FCC Ni matrix or  $\gamma$  matrix. The  $\gamma'$  phase is represented as  $Ni_3(Al, Ti)$ . A volume fraction as high as 70% of the  $\gamma'$  precipitate is needed to strengthen the matrix.

Al, Ti and Ta are used as precipitation-strengthening elements, Cr is used to increase the alloy's resistance to corrosion, Mo and W are used to increase the melting temperature, W, Nb, Mo and Ta help improve the creep strength and Re is added to slow down the coarsening of the  $\gamma'$  precipitates. In equiaxed superalloys C and B are used as grain boundary strengthening elements but they also reduce the microstructure stability at high temperatures. All these elements could also form other phases like  $\sigma$  or  $\mu$  which have undesired side effects [2].

**Comment:** The composition of the superalloy dramatically determines its structure and properties. To understand the role played by each of the alloyed elements, intense experimentation is required. Another method could be using atomistic simulations and molecular modelling to get a better theoretical understanding and only then performing experiments. Such simulations and research is already being done at Indian R&D institutes. Equipping them with better computing power, access to a shared database of experimental and computational data collected by other researchers and availability of material characterisation tools would accelerate the material design process. The significance of such Integrated Computational Materials Engineering (ICME) approach will be emphasised throughout the coming sections.

### 2.1.2 Investment casting

The process of investment casting is also known as "lost-wax casting" and "precision casting". It can cast complex shaped products accurately with a good surface finish. The four key steps involved in the production of turbine blades are : mold production, casting, heat treatment, and thermal barrier coating. The subject of Thermal Barrier Coatings is discussed in a later section.

#### Mold production

In investment casting, a new mold is required to fabricate a new cast each time. And to ensure a good cast a good mold material with some desired properties is needed.

First, a wax mold is created from a master mold. A grain selector is added to the solid wax mold which dictates the crystal orientations for the SX blade. Two kinds of grain selectors are used. A gate or a blocker selector is a pigtail shaped funnel which allows only one orientation of grains into the cast. Another is a crystal seed which is placed with the desired orientation on which the blade grows during casting.

A major challenge is the high reactivity of superalloys with the ceramic shell in molten state. Their extreme reactivity with refractory oxides result in an oxygen enriched surface layer which degrades the property of the cast. Materials for the shell have evolved significantly. In 1981, Terkelsen attempted to cast Co and Ni based superalloys with a ceramic shell made from an inner layer of alumina with silica as binder, and an outer layer of zircon with colloidal silica as binder. This reduced the chain porosity in the cast product [26]. In 1993, Horton prepared a slurry of yttria with colloidal silica as binder. This slurry prevented the growth of defects on the surface of the ceramic shell [10].

Nowadays, slurries containing alumina, silica, zirconia and other binding agents are used to dip the wax structure. The wax mould is then covered with the same particles until the desired thickness is reached. Most often, multiple layers of different properties are pasted together. Then the wax is removed by melting and the investment casting shell is heat treated to strengthen it.

Though the work done by the researchers is satisfactory to some extent, the problem of high chemical reactivity of the super alloys with the ceramic shell still persists.

**Comment:** There are many unknowns in the process. For example, What are the particular slurry compositions? What is the binding agent? What heat treatment processes and what thermal gradients should they follow? The complexity in developing a good ceramic mold does not lie in slurry composition selection but in the heat treatment process to get the desired properties. This is majorly an experimentally resolvable challenge. The pigtail shaped grain selector funnel pose a design challenge. Research in this area is not seen.

#### **Investment casting**

The method used is called the Bridgman process, where the mould is cooled by moving it across a high temperature gradient. The directional cooling due to the transfer of the mould from a region of high to low temperature ensures directional solidification. Further details can be found in [9] and [15].

Improvements in the productivity of SX casting is achieved in liquid metal-cooling assisted casting (LMC). This process is able to achieve larger gradients of temperature and thus an increment in the size of the cast. Another process used to cast SX blades is called gas cooling casting (GCC). Both the LMC and GCC process cool the entire cast aggressively and various inhomogeneties arise in the process. Therefore the Bridgman process is the one industrially used to cast SX alloys till date [9].

**Comment:** This is the critical challenge in developing single crystal turbine blades. An academic understanding of the Bridgman process has existed for a few decades but very little could be practically achieved. The size of the turbine blades also pose an additional challenge in it.

#### **Heat treatment**

The heat treatment processes include homogenization, solutionizing, aging etc. These processes vary depending on chemical composition, fabrication routes, and intended service conditions. Homogenization is done to recrystallize the microstructure, Solutionizing dissolves age-hardening constituents and carbides into the solid solution. Ageing is done to drive the precipitation of the  $\gamma'$  phase throughout the blade [5] [24].

**Comment:** The heat treatment process fine tune the microstructure of the SX blade. This area of multi phase microstructure evolution under heat treatment is being researched. The mentioned ICME initiatives would significantly accelerate our understanding. Building the equipments for such processes with the existing theoretical understanding is difficult, but work on both has to be done simultaneously so that theories can learn from experiments and vice versa.

### **2.1.3 Failure Modes**

Material selection, blade design and its integration with the engine requires an in-depth understanding of the failure modes of turbine blades. This section presents a summary of such mechanisms.

From the study [18], it was found that the significant damage to the blade is caused during throttle movements of the aircraft. Other factors such as cruising Mach number, altitude and average day temperature also play a role in damaging the blade. The role played by each factor is not completely understood.

#### **Fatigue**

The effect of blade crystallographic orientation and temperature on its integrity has been studied for many Ni-base superalloys. It was found that the different orientations

of SX turbine blades display different low-cycle-fatigue (LCF) life, but does not influence high-cycle-fatigue (HCF) life [3]. Also, an uniform distribution of  $\gamma'$  precipitates improves the fatigue resistance of the blade [32].

### **Creep**

Creep strength depends on the volume fraction, morphology, distribution and average size of  $\gamma'$  precipitates [6] [7] and on the elastic modulus and misfits of the  $\gamma/\gamma'$  interface. The primary determinant of degradation of creep strength is  $\gamma'$  precipitate coarsening during prolonged thermal exposure [1].

### **Hot corrosion**

The rate of hot corrosion is significant for metal temperatures above  $900^{\circ}\text{C}$ . Generally sulphate deposition on blade surface initiates hot corrosion. The rate is determined by: rate of deposition, material of the deposit, temperature of the metal and the chemical composition of the environment.

Two kinds of hot corrosion failures can happen in an SX blade [2]. Type I hot corrosion which occurs around  $750\text{--}900^{\circ}\text{C}$ , and Type II hot corrosion occurs around  $600\text{--}800^{\circ}\text{C}$ . Elements like S, Cl, alkali metals, Zn, Pb can cause significant damage to the metal. Concentration of gases like  $\text{SO}_2$ ,  $\text{HCl}$  and even water vapor has considerable affect on hot corrosion.

It is clear that coated SX blades corrode far less than un-coated SX blades.

**Comment:** The different mechanisms of SX-blade failure are academically well understood. What remains is how to control the failure-behaviour with heat-treatment processes, composition, blade design etc. Usually data from failure analysis at lab scale experiments is extrapolated to predict real-world behaviour. But a better scientific approach would be to have a demonstrator engine. New blade materials/designs could be integrated with such an engine and tested by running it in a wind tunnel or flying it on a demonstrator aircraft. The failure data collected in this manner would be much more useful.

#### **2.1.4 Rhenium and its significance**

Of all the elements alloyed in an SX blade, the most expensive is Re. It provides incredible strength to the blade at higher temperatures. It accounts for 3-6 wt.% but its costs about 10 times the rest 97% of materials.

**Comment:** Rhenium is expensive. Countries like US have already started looking for other elements/compositions with that provides the necessary properties without it.

## **2.2 Gamma Titanium Aluminides**

This section presents a summary of the material and fabrication processes associated with development of  $\text{TiAl}$  alloys for applications in the jet engine.

The principal advantages of TiAl-based alloys are low density ( $3.9\text{--}4.2\text{ g/cm}^3$ , depending on composition), high specific strength, high specific stiffness and improved creep, oxidation resistance, and burn resistance (in comparison with conventional titanium alloys) properties up to  $800^{\circ}\text{C}$ . Its specific 1000h rupture strength and its specific strength are superior to those of conventional titanium alloys, alloy steels or Ni-based super-alloys for the entire range of temperatures from room to  $800^{\circ}\text{C}$ . While its high temperature properties are strong, its poor room-temperature ductility is the major barrier to its applications as structural components [30].

The GENx engine is the first commercial aircraft engine that has its low-pressure turbine made of the Ti-Al alloy 4822 [4].

### 2.2.1 Material design:

Al content in TiAl alloys is generally between 44-48%, the optimum concentration for high temperature strength is 46%. For low Al content, at high temperature, the  $\beta$ -phase forms which makes the alloy hot machinable but spoils the creep properties.

The second generation of TiAl alloys had a composition like the GE alloy *Ti-48Al-2Cr-2Nb* and the ABB alloy *Ti-47Al-2W-0.5Si*. Then higher levels of Nb and Mo were introduced to have better high temperature capabilities up to 850°C which are considered to be the third-generation [4].

Nb could be added in small amounts to increase the oxidation and creep resistance. It also increases high temperature strength if added between 5% and 10%. The state-of-the-art TiAl alloys developed by Plansee, Austria and GKSS Research Center, Germany contain 10% Nb. Alloying of Ta, W, C, Mo, Cr (<8%) increases the oxidation and creep resistance. V, Mn, Cr increases ductility and B reduces the grain size [16].

It is generally accepted that a base composition of Ti(45-46)Al(4-8)Nb with minor additions (of C and B) offers the best properties [30]. Unlike most TiAl alloys TiAl 4822 possesses high fluidity and good castability [4].

**Comment:** The optimum base composition of TiAl alloys is known. The influence of minor additions of certain elements on its properties has also been studied to some extent but not specifically for jet engine applications. Here the major challenge is the alloying process itself. As TiAl has poor ductility, there is a trade-off between its machinability and high temperature properties. Studies on properties with minor composition variation are required.

### 2.2.2 Production

Investment casting, ingot metallurgy (IM), and powder metallurgy (PM) are popular techniques that have been used to produce TiAl parts. More recently, advanced techniques such as direct rolling, laser forming, and mechanical alloying have been investigated with good success. Several rapid sintering/consolidation techniques such as plasma pressure compaction, spark plasma sintering, pulse discharge sintering, high density infrared processing and explosive consolidation have also been successful in forming TiAl with desired mechanical properties [16] [4].

The major drawbacks in production of TiAl alloys is their extremely low ductility and high processing temperature. Processes to fabricate materials with such low ductility are still not fully developed. The high processing temperature demands the processing tools to themselves have good high temperature properties.

Casting still is the most cost-effective process to manufacture complex shaped products. The challenges include the reactivity of molten TiAl to the ceramic mold and defects such as shrinkage and porosity. High reactivity demands the usage of cold walled crucibles which bring their own set of challenges. The low ductility comes from the large lamellar grain structure. The fact that addition of Boron decreases the grain size was discovered almost 35 years ago. Though its an effective technique, the formation of borides lead to decrease in fracture toughness of the alloy [30].

**Comment:** The reaction of TiAl with the ceramic mould poses a challenge. Since neither the composition, nor the processing temperature of the alloy could be changed, we



need to search for better ceramics for the mould. Again, intense experimentation aided with computational tools is required.

### **Ingot metallurgy**

Ingot metallurgy and casting routes involve producing TiAl ingots and castings by skull melting. The resulting microstructure of the ingots is characterized by large columnar grains consisting of chemical inhomogeneities, and segregation. Improvements in the microstructure can be achieved by thermo-mechanical processing and recrystallization [11].

To have a chemically homogeneous alloy, the melt produced has to be free of impurities. Therefore, processes like vacuum-arc-melting and cold-hearth plasma arc melting are employed instead of skull melting.

**Comment:** Here again we emphasise on the significance of the post-cast heat treatment processes. High temperature furnaces and quenching methods need to be developed. Repeatability of such a casting process demands an in-depth theoretical understanding of microstructure evolution and real-time low-latency control on the cast environment.

### **Powder metallurgy**

Many of the problems associated with ingot metallurgy (IM), such as center-line porosity, chemical inhomogeneity, regions of varying density and microstructure can be solved by powder metallurgy. Further, powder metallurgy enables the development of new alloys that cannot be made by conventional ingot metallurgy [31].

The general route in PM is, first gas atomization of pre-alloyed powder and then consolidation using hot-isostatic pressing. Mechanical alloying of element powders is possible but the threat of purity from contamination by milling media and container is a challenge yet to overcome.

Hot-isostatic pressing is generally used to form TiAl billets. Some of the post processing steps after hot isostatic pressing involve hot extrusion, isothermal forging and hot rolling to sheets. Its disadvantage being that the TiAl powder has to be exposed to high temperature and pressures for a long duration which leads to grain growth. The process cannot offer any controls on the final grain size [16].

The PM route is found to be more cost effective than the ingot casting process [16].

**Comment:** Powder metallurgy processes, though not the cheapest of methods, operate at a lower temperature than ingot casting processes. They are still not developed for industrial applications.

## **2.3 Thermal Barrier Coatings (TBCs)**

TBCs are applied on the turbine blades to shield the alloy from the high temperatures of the gas, to protect it from impacts of particulate matter present in the atmosphere and prevent hot corrosion. TBCs are applied in three layers: Bond coat, Thermally grown oxide layer and the ceramic top coating [19].

### **2.3.1 Material design:**

The TBCs consist of a top ceramic coating, a middle layer of a thermally grown oxide (TGO) and a bond coat.

Thermal insulation is provided by the top-coat which is yttrium oxide ( $Y_2O_3$ )-stabilized zirconium oxide ( $ZrO_2$ ) or YSZ. YSZ displays a variety of desired characteristics which makes them perfect for top-coat applications [14]. The two methods used to produce YSZ are atmospheric plasma spray (APS) [28] and electron-beam physical vapor deposition

(EBPVD) [13]. EBPVD is preferred over APS as it produces a smoother surface, a columnar grain structure and improves corrosion resistance [2].

The ceramic coating offers the maximum temperature gradient. YSZ has very low thermal conductivity due to its high concentration of point defects which helps scatter the heat phonons. It also has a relatively high thermal expansion coefficient that helps alleviate the mismatch between it and the base metal. To further alleviate the mismatch stresses, defects are introduced [20].

Although  $ZrO_2$  can be stabilized by a range of different oxides,  $Y_2O_3$  has been found to be the best for TBC applications. YSZ exists in three different polymorphs monoclinic, tetragonal and cubic depending on composition and temperature. Addition of 7 – 8%  $Y_2O_3$  produces the optimum microstructure [20].

The bond coat is composed of MCrAlY (M: Co, Ni), which is used to further reduce the heat penetration and relieve the stresses that raise due to different thermal expansion coefficients of the component alloy and the top ceramic coating. Because the top ceramic coat has high oxygen penetration properties, a layer of oxide (TGO) grows on the surface of the bond coat. The TGO layer is stabilized by the formation of  $\alpha - Al_2O_3$  that protects the inner layers from further oxidation. The layer also acts as an adhesive between the top coat and the bond coat [19][29].

**Comment:** We see a number of constraints on the material selection for top and bond coats. From rate of oxidation to thermal expansion, all properties if were to be experimentally tuned will require significant time and resources. Here computer aided material selection methods will cause notable acceleration. Details of such a method is discussed in a later section.

### 2.3.2 Deposition techniques

Before any TBC layer can be applied the SX blade surface needs to be roughened. It is achieved by a process called grit blasting in which hard angular particles are blasted onto the blade surface which not only cleans it but also increases the surface area.

TBCs have different deposition techniques depending on the temperature and material used. When choosing a TBC process, many aspects including performance, capital, process cost per part, thickness, composition, surface roughness requirements, and cooling hole cover should be considered [29]. The deposition processes widely used are electron beam-physical vapor deposition (EBPVD), chemical vapor deposition (CVD), and atmospheric plasma spray (APS).

#### Electron beam physical vapor deposition

In the EBPVD process, an YSZ ingot is evaporated using an electron beam in a vacuum chamber. The component surface which should already have a bond coat is preheated in a low oxygen environment at about  $1000^{\circ}C$  to have a thin TGO layer grown on it. The vapor cloud of the YSZ is then used to coat the surface. The temperature of the surface component is kept at about 0.47 times the temperature of the YSZ vapor to ensure adhesion. The EBPVD process produces columnar microstructure in the TBC layer [25].

#### Chemical vapor deposition

In the CVD process the surface is exposed to the vapor of the material which is to be deposited on it. The vapor material undergoes reactions with the surface alloy and gets deposited. The deposition rate is extremely low, about  $10\mu m h^{-1}$ . Research has shown that other energy sources like plasma and lasers could increase the deposition rate significantly. The newly developed laser CVD could be particularly attractive to obtain high deposition rates as high as  $660\mu m h^{-1}$  [27].



### Atmospheric plasma spray

In the APS process, gases like *Ar*, *He* and *N<sub>2</sub>* are converted into plasma and a high speed plasma jet is used as the heat source. Because of the plasma speed, the coat material sprayed on it collides with the surface at high speeds and thus gets deposited. The disadvantage is that the air/gases in the plasma is incorporated into the structure which makes it porous and there is the possibility of formation of oxides and nitrides depending on the coat material [21].

**Comment:** Among the deposition processes, the most promising one is the EBPVD process. Significant developments in CVD is required to achieve a sufficient deposition rate for industrial purposes. At a lab scale, EBPVD equipment are available but not for the industrial scale. Even here, more than development of the equipment the challenge is in achieving the desired properties though fine-tuning the environment parameters.

### 2.3.3 Coating failure

The growth of oxide layer on the bond coat is the major reason for TBC failure [19]. The mismatch in physical and thermal properties of the oxide layer and the bond coat develops stresses as the oxide layer grows, which could increase the porosity of the layer enhancing oxidation and lead to complete failure. The failure mechanisms for EBPVD TBC and APS TBC are quite different. Overall EBPVD TBCs are more resistant to failure than APS TBCs [2].

**Comment:** The growth of oxide layer is inevitable. For it stay within a critical width, we must look into different compositions and pairs of the top and bond coat. Huge data has to be collected experimentally on these compositions and properties. Computational analysis in this sector is not very accurate.

With this we end our discussion on the technical details of materials designs and manufacturing. We present in the next section a summary of the identified challenges and propose potential industry/laboratory partners to work toward a resolution.

## 3 Identified challenges and resolutions

From the brief-technical summary on materials design and manufacturing we can classify the identified challenges into the following classes according to their resolution methods.

1. Database - India's lack of an indigenous materials database.
2. ICME - challenges in materials modelling and simulation.
3. Experiments - challenges in experimental methods.
4. Equipment manufacture - our inability to manufacture characterisation, testing, synthesising equipment etc.
5. Infrastructure - challenges at an organisational scale.

Below, we discuss each of them in detail except the challenges in infrastructure.

### 3.1 Database

Data on materials properties is expensive. A typical thermodynamic database for steel costs around 10 Lakhs per annum. Data on superalloys is even more expensive. Cost is not the only issue. Data on materials critical to national-security is classified by the host nations and is kept secret by the private companies. It is impossible for us to have even limited access to such a database.

Databases have proven to dramatically reduce the time and cost of developing advanced materials. Databases include

1. **Experimental databases :** Databases populated with a wide variety of materials data with varying parameters. They aid in identifying a material system from a set of desired properties and also serve as the base on which computational models are built and tested.
2. **Thermodynamic and Kinetic databases :** Databases containing the thermodynamic and kinetic parameters like Gibbs energy  $G$ , mobility  $\mu$  etc for every material system of interest. Though data on single component Such data can be generated experimentally as well as computationally. This information is a necessity for designing the manufacturing processes of any material system.
3. **Materials property databases :** Data on many physical and chemical properties can be computed with atomistic modelling, molecular dynamics simulations, DFT etc. And due to its computational nature, there is not limit (except theoretical) on the variety of material systems on which this method can be applied.

India has a significant number national laboratories and academic institutions to create a database of its own. Such an endeavour requires minimal investments of servers, computer science engineers and a high-speed network of institutions. The National Knowledge Network (NKN)\* is already connecting the institutions and national laboratories. And developing a database from the available information is not at all difficult for an Software-oriented nation like India.

We present here a simple collaborative model for building a national database:

- **Data collection:**

1. MIDHANI - Composition microstructure correlations of superalloys and Ti alloys. Their solidification kinetic and thermodynamic data, data on post-cast heat treatment processes and data on processing equipment and control.
2. DMRL - Complete infancy-to-product data on synthesis superalloy components.
3. Other labs - data on physical properties (strength, creep, fatigue etc.) could be collected from available literature and by experimentation with small-scale samples.

- **Data processing:**

1. IITs + IISc : could invest a portion of their supercomputing resource on processing of raw experimental data collected in part 1. The processing converts the raw data to mathematically useful data for modelling, simulation and further analysis.
2. TATA Adv. Systems Limited could be involved in database building and data processing for their common interest in this area.

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\*More about NKN in <https://nkn.gov.in/en/>

- **Database :**

Creation and maintenance of a database will require an independent organisation to oversee updates and repairs.

## 3.2 ICME

Integrated Computational Materials Engineering (ICME) has significantly accelerated the process of materials design and development in the past few decades. Our ability to simulate solidification, deformation, re-crystallisation, ageing etc has aided our experiments and made the manufacturing processes more efficient.

Having said that, it is important to mention the significance of experimental data to serve as the validation dataset, in the development of computational models. All the areas in which ICME is to be implemented, a corresponding experimental lab has to be set up.

In regard to materials development for a jet engine, the enlisted areas are where ICME can accelerate growth are:

### 3.2.1 Material selection/design

To design the optimum material for the desired application, first we need to understand the composition-property correlation in materials. Each element added to a Ni-base superalloy has a functional advantage and some disadvantages. Due to the advantage-disadvantage trade-off only a particular concentration gives the optimum property. This process gets highly complicated for multi-component systems and is extremely resource intensive to be carried out experimentally.

Here first-principle methods like, atomistic modelling, molecular dynamics, DFT etc can be implemented to gain a basic understanding of the stability and physical and chemical properties of the material system with varying composition. A set of compositions can be selected from this analysis for further experimental investigation.

Within the domain of Jet Engine materials design, some areas are where ICME could accelerate development are:

1. What set of elements could be added at what composition to improve the machinability/room temperature ductility of TiAl?
2. What set of elements can be used as a substitute for Rhenium *Re* in Ni-base superalloys?
3. What are the most suitable materials for top-bond coat pairs for TBC application? Suitability in terms of high temperature stability, strength, thermal expansion etc.

### 3.2.2 Synthesis

We saw two major problems in material synthesis. The Bridgman process for single crystal casting of superalloys and the powder metallurgy sintering of TiAl powders. Both processes are academically understood and can be replicated at a laboratory scale. Their scaling to an industrial scale is still an unsolved problem.

The Defence Metallurgical Research Laboratory (DMRL) has recently succeeded in development of SX-blades for Helicopter engine applications<sup>†</sup>. It is an impressive milestone but there is a long way to go.

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<sup>†</sup>link to DMRL's site

Developing the casting process for SX blades and sintering process for TiAl is majorly an experimental work. But as experimental trials are resource intensive, a major portion of it can be outsourced to ICME methods (modelling and simulation).

In regard to synthesis, the areas where ICME could accelerate development are:

1. Find the range of environment variables (eg: Temperature gradient) under which the Ni-base superalloy undergoes single crystal growth.
2. Develop multi-component models of TiAl consolidation under sintering.

### 3.2.3 Post-cast heat treatment

The post-cast heat treatment processes are what refines and strengthens the microstructure.

### 3.2.4 Failure analysis

Ni-base superalloys contain a variety of elements at various compositions. Minor additions of some elements to the base composition of TiAl changes its properties

- Understanding Ni-base superalloys single crystal synthesis. The processes of solidification, growth and microstructure evolution under heat treatment.
- Understanding consolidation of TiAl powders in sintering and the influence of post-cast heat treatment processes on TiAl microstructure.
- Search for a Rhenium (*Re*) substitute for superalloys.
- Designing the pig-tail shaped grain selector for SX casting.
- Modelling failure behaviour of engine components.
- Selection of top-bond coat material pairs for TBC applications.

## 3.3 Equipments

Temperature control is the major challenge in building a Single crystal casting equipment. How a particular temperature is achieved in a furnace, its time-dependent fluctuations determine directly the microstructure of the cast.

Here improvements can be made by

- Understanding how the temperature varies during the process at the mould surface.
- Building better temperature controls.

## 4 Opportunities for IITM

From the above discussion we understood the challenges and potential resolutions to the materials aspect of the jet engine problem. Now, we enlist a few collaborations and problem statements that will work towards making progress in overcoming the challenges.

Institution	Reason	Challenge
Defense Research and Development Organisation (DRDO)	<ol style="list-style-type: none"> <li>1. GTRE - development of the Kaveri engine.</li> <li>2. DMRL - development of critical material technologies for the jet engine.</li> </ol>	<ol style="list-style-type: none"> <li>1. DMRL - ICME aided development of SX superalloys. Scaling the synthesis processes to an industrial scale.</li> <li>2. DMRL - Data collection on synthesis and processing of superalloy components.</li> <li>3. GTRE - Solving the performance problem at high altitude and low thrust generation.</li> <li>4. GTRE - Resolving the combustion challenges with NC-CRD.</li> </ol>
CSIR National Aerospace Laboratories (NAL)	<ol style="list-style-type: none"> <li>1. It has manufactured composite structural components for HAL tejas.</li> <li>2. It offers standard modulus grade carbon fibre technology.</li> <li>3. It can manufacture C/SiC and SiC/SiC composite products through Chemical Vapor Infiltration Process.</li> <li>4. Involved in development of TBC for missile components.</li> </ol>	<ol style="list-style-type: none"> <li>1. Development of composite casing and fan blades for the engine.</li> <li>2. Development of high temperature composites for static components of the engine. Eg: combustion chamber, exhaust nozzle etc.</li> <li>3. Development of Carbon-Fibre fan-blades.</li> <li>4. Development of TBCs.</li> <li>5. Development of Physical Vapour Deposition process for TBC coating of engine components.</li> </ol>

CSIR Advanced Materials and Processes Research Institute (AMPRI)	1. It is involved in the development of Al Metal Matrix Composites (MMC) and Foams.	1. Development of high temperature MMCs for static component application.
MIDHANI	1. Manufactures alpha, near alpha, alpha + beta classes of Ti alloys. 2. Manufactures vacuum induction casted equiaxed superalloys - INCONEL , NIMONIC and Hastelloy class of superalloys	1. Data collection on casting and post-cast treatment processes of Ti alloys and Superalloys. 2. ICME aided scaling of existing processing technology at MIDHANI for large-scale manufacturing of engine components. 3. Development of the SX casting process.

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