Project Details

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<th>Project Title</th>
<th>Design of aluminide bond coats for low pressure jet engines using diffusion kinetics and high-performance computing approach</th>
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| Project Summary | Low pressure turbine blades use titanium aluminide (Ti-Al) based lightweight structural alloy in jet engines because of its high specific strength and good creep strength up to 1100 °C. However, a major challenge lies in its poor oxidation resistance at an elevated temperature. To be enable to operate TiAl based engines at higher temperatures, thermal barrier coating is applied over it. Such a coating comprises of a ceramic topcoat for thermal protection, and an aluminide bond coat to ensure good compatibility between the underlying TiAl alloy and ceramic overlayers while supplying aluminium to promote a thermally grown oxide (TGO) for oxidation protection. *Therefore, there is a pressing need to develop a suitable aluminide bond coat for TiAl to enhance its service life in pursuit of better thermal efficiency without compromising its intrinsic structural properties.*

   Chemical alloy modification is one of the techniques to develop a bond coat alloy. The effects of chemical alloying of various refractory elements in the Tialuminide phases will be studied with an emphasis on investigating the kinetic behaviour of oxidation and development of interdiffusion zone at the bond coat–TiAl interface. The kinetics of the phase development will be explored by quantifying the atomic transport of primary components, Ti and Al, using various diffusion models. The atomic transport is dictated not only by the thermodynamic potentials of the atomic species for different phases under consideration, but also a function of the defect chemistry of those phases.

   Another challenge encountered with such a conventional alloy design technique is long processing times, and indeed are time consuming (requiring methods such as trial and error in the composition-temperature domain). In this collaborative project, we envision to draw the benefits from the advances made in the area of high-performance computing (HPC) to accelerate the process of alloy designs; thereby addressing the inherent combinatorial explosions that one faces in the design choices while fabricating alloys. In particular, known discretisation of the phase development and transport equations already exist. Thus, using the already available algorithms which compute the solutions to the above-mentioned discretised equations, one can possibly create the model of computation for the atomic transport phenomena that takes place at the bond coat-superalloy and bond coat-oxide. |
interfaces, and run the model against a set of sought properties that one desires to investigate.

Therefore, a Kirkendall marker based diffusion study integrated with the high performance computing can help to develop a novel bond coat for the TiAl system.

### PhD Supervisors

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<th>Role</th>
<th>Faculty</th>
<th>Academic Unit in IITD</th>
<th>Email ID</th>
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<tbody>
<tr>
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### Project requirements (Student qualifications, experience required, etc)

- B.Tech/M.Tech/M.Sc in either Materials Engineering or Materials Science preferably, or Mechanical Engineering with an experience in the computational related area.
- Expertise in any of the microscopy tools would be preferable.
- (Preferable) Programming experience in C/C++ or Java.
- Ready to join as a full time PhD student.

### Source of funding (IRD/FITT Project details, if any)

Candidate should have his/her own fellowship from CSIR/UGC.

### Role of Faculty Members involved:

- Faculty member, Dr. Sangeeta Santra, has research expertise in solid-state diffusion, thermodynamics and kinetics of various multi-material systems. She has an experience on understanding the correlation of microstructure-property with a key focus on thermodynamic potential changes at the interfaces. She will supervise the PhD student for the diffusional based calculations and other relevant experimental work.
- Faculty member, Prof. Subodh Sharma, has research expertise in High Performance Computing (HPC) and parallel programming with GPUs. Prof. Sharma will undertake the supervision of the joint PhD student on topics such as discrete computation modeling of diffusion-based calculations and mapping the tasks efficiently on high performance CPU machines with GPU co-processors.