Materials Selection, Modeling and Mechanical Design

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ABSTRACT

These lecture notes address materials and structures issues associated with the MIT Microfabricated gas turbine engine. An overview of the project and the performance goals is provided. These are translated into requirements for the materials and structural design. Particular emphasis is provided on the approaches taken to designing with brittle materials at low temperatures and designing with ductile creeping materials at high temperature. A novel approach to structural reinforcement using SiC in combination with Si is introduced.

1.0 INTRODUCTION

This lecture will provide an overview of material selection, structural design and the requirements for material and structural models motivated by the MIT Microengine project. This project has been running since 1994, and is motivated by opportunities for small scale propulsion and portable power generation. The key guiding principles of the project are:

1) µfabrication of high strength and/or refractory materials enables the concept of high-power density µsystems (mm scale): µgas turbine engines, µrockets, µcompressors, µpumps, µhydraulic pumps/energy harvesters, µrefrigerators.
2) Power densities can approach those of full-sized prime movers and power generators (100 W/cc).
3) Cost could be very low given sufficient demand (10^8 units/year).
4) Power microsystems could be an enabling technology for new concepts: Portable power, propulsion, cooling, flow control.

In addition to the microengine several other projects using microfabrication processes have been initiated at MIT, some of which are shown as images in figure 1.

Spearing, S.M. (2005) Materials Selection, Modeling and Mechanical Design. In *Micro Gas Turbines* (pp. 8-1 – 8-16). Educational Notes RTO-EN-AVT-131, Paper 8. Neuilly-sur-Seine, France: RTO. Available from: http://www.rto.nato.int/abstracts.asp.

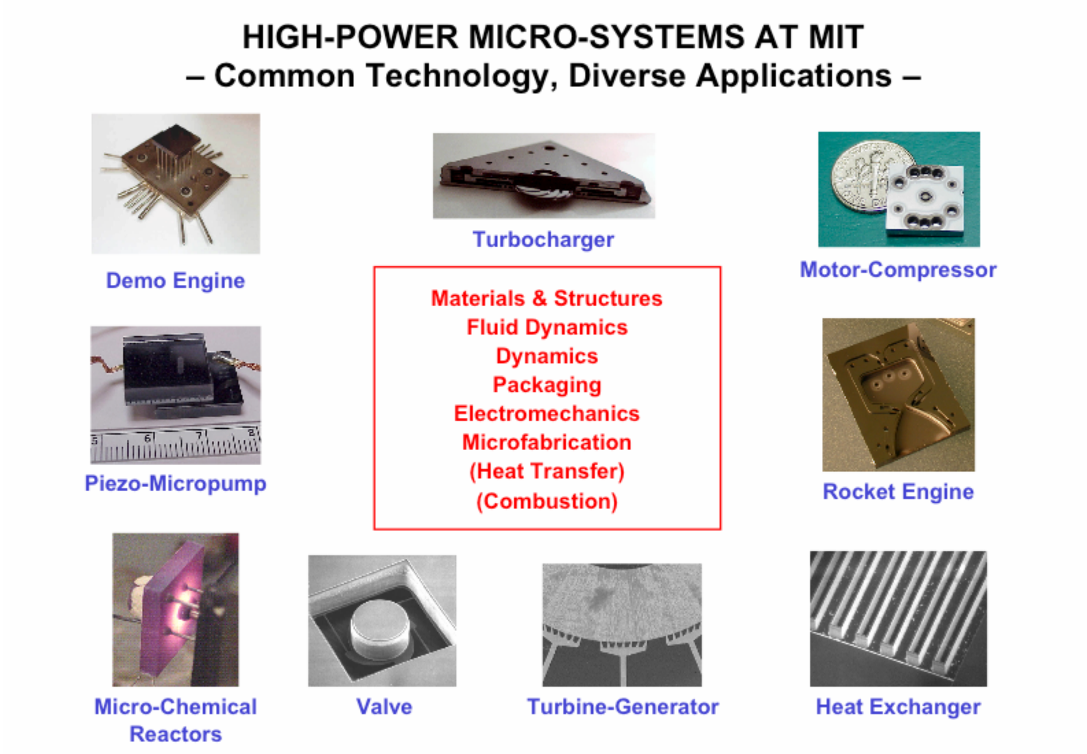

Figure 1: Images showing Microfabricated Devices and Components.

In order to realize these devices there are certain physical requirements that must be met:

1) High peak cycle temperatures (1600-2500 K), which translates into a requirement for high temperature materials.
2) High peripheral speeds (400-600 m/s). Which implies highly stressed rotating parts (100's of MPa). Note: rotor power density is proportional to (tip Mach No.)^2 which in turn is proportional to stress.
3) Low friction bearings (air bearings for µengine): Avoid sliding contacts at all costs.
4) Reasonable component efficiencies which implies a requirement for close tolerances (better than 1 µm).

Requirements 1) and 2) have implications for the chosen materials and items 3) and 4) for the processes used. These requirements and the coupling between them provides the motivation for the two lectures in this series.

The device shown in figure 2 is sized to have the following performance metrics: Thrust = 11 g, Fuel burn = 16 g/hr, Engine weight = 2 grams, Turbine inlet temp = 1600 K,Rotor speed = 1.2 x 10^6 RPM, Exhaust gas temp = 970°C. The initial demonstration device is entirely fabricated using silicon. This results in relatively poor performance for the engine, due to the temperature restrictions on silicon, however, it exploits relatively mature microfabrication technology. The key process steps are the extensive use of high precision deep reactive ion etching, and wafer bonding to create the three dimensional structures. The bond lines can clearly be seen in figure 2. Figure 3 shows a complete engine. Figure 4 shows a die with fluidic connections. Packaging is a very important topic for such devices, but is outside the scope of this talk. If interested please refer to other references on the subject [1].

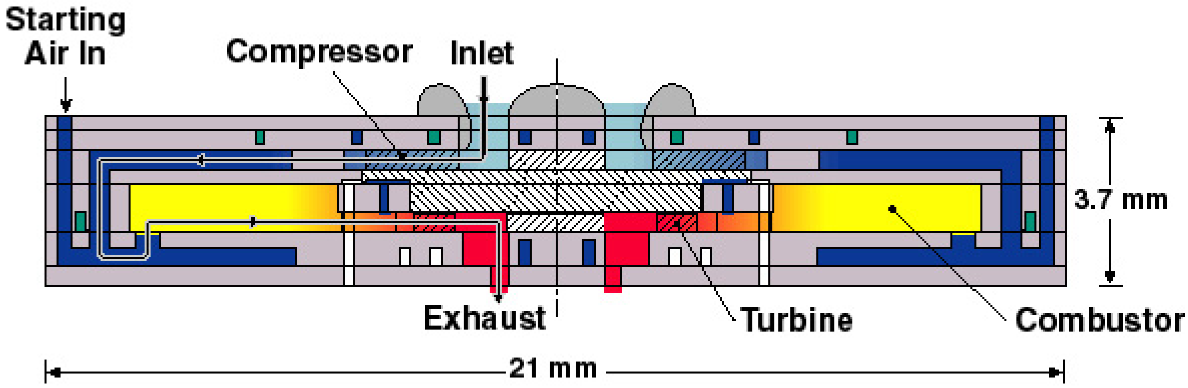

Figure 2: Cross-Sectional Schematic of MIT Microengine.

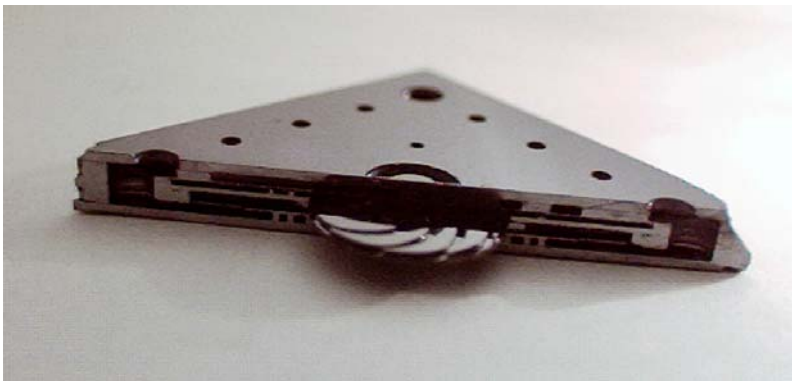

Figure 3: Cross-Sectional Schematic of MIT Microengine.

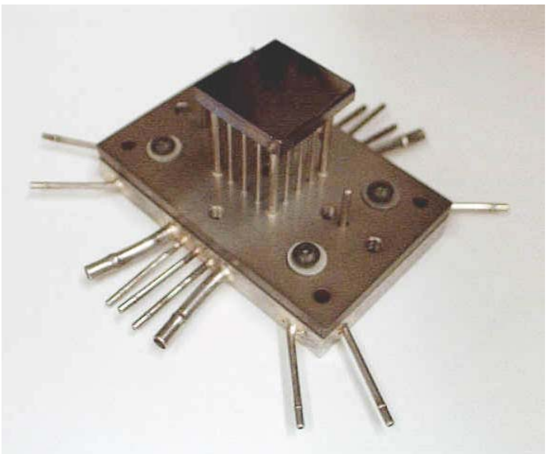

Figure 4: Packaged Microengine. Kovar tubes and glass frit bonding are used to bring fuel to the engine die.

2.0 MATERIALS AND STRUCTURES CHALLENGES

In the course of pursuing the microengine and other power MEMS project several recurrent themes emerge as particular challenges in the realm of materials and structures:

1) The effects of scale – quasi-fundamental, mechanism-dependent, indirect.
2) Characterization of materials at appropriate scale, geometry.
3) Overall structural design process in uncharted design space: Constitutive laws, probabilistic design, heat transfer.
4) Development of µfabricatable refractory structures.
5) Insertion of functional materials – piezoceramics, SOFC electrolytes, catalysts.
6) High precision deep etching of high strength structures.
7) Creation and characterization of high strength wafer bonds.
8) Engineering of thick (10-100 µm) high integrity deposited layers (SiC, SiO_2).
9) Packaging – CTE matching, joining, heat transfer.

The subject matter of this lecture will focus on items 1, 2, 3 and touch on 4. The following lecture will cover items 6, 7 and 8. Issues of functional materials integration can be found elsewhere [2, 3].

2.1 Effect of Scale

The following points are worth bearing in mind when considering the effects of scale on the materials and structures aspects of microengine design:

1) Overall concept is enabled by favourable cube-square scaling (power, thrust, scales with area, mass with volume).
2) Stress levels are scale-independent – continuum mechanics.
3) Structural configurations are dictated by fabrication, system considerations: (a) Reduced ability to tailor for stress uniformity. (b)Increased sensitivity to deformations (tolerances).
4) Materials are brittle – high strength at small scale (GPa strengths routinely achieved).
5) Thermal shock not a concern.
6) Surface effects (oxidation) potentially of increased concern.
7) Creep and yield largely unaffected (at 100 mm – 10 mm scale), although use of single crystal silicon introduces challenges.

2.2 Material Selection

Material selection for the microengine was driven largely by the need to create a working device within a limited time scale. In order to achieve this, a conscious decision was taken to minimize programmatic risk associated with introducing new materials and developing new processes. As a result the first generation, demonstration engine has been largely made out of silicon. Nevertheless the material indices for microfabricated silicon compare quite well with those for the metal alloys used in macroscale gas turbine power plant. Figure 5 shows the relevant performance indices for turbomachinery. The relatively low density of silicon and its high strength and stiffness make it an attractive material for rotating structures. Even its relatively poor temperature capability can be accommodated with careful design. However, the opportunity for introducing more refractory ceramic materials is clear from this figure.

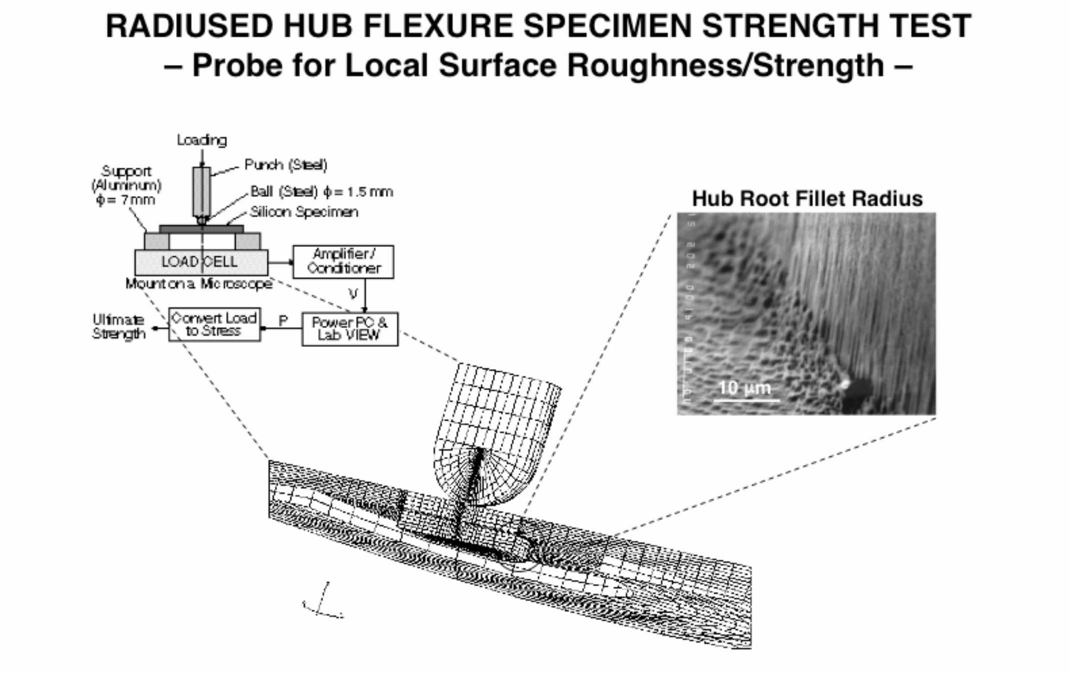

Figure 5: Radiused-Hub Flexure Specimen Strength Test.

Table 1: Selected Performance Indices and Materials Relevant to Macro and Micro-Gas Turbines

MICRO vs. MACRO MATERIAL PROPERTIES

	Ni-based Super Alloys	Titanium Alloys	Macro (Micro) Ceramics	Micro Silicon
Centrifugal Strength [$\sqrt{\sigma_f/\rho}$] (m/s)	330	420	420 (670)	1000
Thermal Strength [$\alpha E/\sigma_{f/y}$]	2.7×10^{-3}	1.2×10^{-3}	2.0×10^{-3} (1.1×10^{-3})	0.9×10^{-3}
Stiffness [E/ρ] (MPa/Kgm^{-3})	~26	~25	~95	~70
Max Temp (°C) limiting factor	~1000 (creep)	~300 (strength)	~1500 (oxidation)	~600 (creep)

3.0 DESIGN FOR ROOM TEMPERATURE STRENGTH

3.1 Mechanical Testing

Given that silicon is a brittle material design for room temperature operation must account for the stochastic aspects of the strength. Axisymmetric flexural specimens were preferred for this purpose, in which the specimen is supported around its edge and loaded centrally [4]. This arrangement avoids extraneous flaws introduced at edges affecting the strength. A modified micro-hardness indenter was found to be very useful for this purpose. Specimens consisted of square die, 10mm x 10mm which were placed over a hole of diameter 5mm – 8mm. A load was applied centrally and the load at fracture recorded. Data such as that shown in table 2 was obtained. Weibull analysis was applied to reduce the data, and obtain the Weibull reference stress and Weibull modulus to characterize the strength distribution.

Table 2: Data from Planar Biaxial Flexure Tests

	Mechanically Ground (A)	Mechanically Ground (B)	KOH Etched	Chemically Polished	STS DRIE
Sample Size	19	30	25	4	20
P-P Surface Roughness	~3 µm	~1 µm	~0.3 µm	~0.1 µm	~0.3 µm
Reference Strength, σ_0	1.2 GPa	2.2 GPa	3.5 GPa	>4 GPa	4.6 GPa
Weibull Modulus, m	2.7	3.4 – 4.2	7.2 – 12	?	3.3

A particular concern for the design was the introduction of flaws by the deep reactive ion etching process. Additional surface roughness was observed at the intersections between horizontal surfaces and vertical etched walls. Since these locations also represent stress concentrations, locally reduced strength was of particular concern. To investigate this issue a novel test specimen was developed: The Radius-Hub Flexure Specimen, which consists of a central hub defined by deep etching. The nominal stress concentration at the interface between the hub wall and the horizontal surface is calculated based on the nominal radius of the fille and used to define a nominal local strength. A schematic of the specimen and details of a typical fillet is shown in figure 6. Data from such tests is shown in table 3. The effect of the locally increased roughness has a significant effect. The reference strength obtained from STS DRIE specimens drops from 4.6 GPa in table 2 to 1.45 GPa in table 3. However, use of a secondary, "smoothing" etch is shown to be very effective in recovering much of this strength loss. An isotropic SF6 plasma etch recovers the local strength to 4 GPa. Such a strength recovering etch is essential if microengine rotating parts are to be able to achieve the high speeds required for power production.

Table 3: Data from Radius Hub Flexure Tests

	STS DRIE	DRIE + Wet Isotropic Etch	DRIE + SF_6 Plasma Etch
Specimen Size	20	16	18
Polishing Thickness	NA	~1.8 mm	~2.7 mm
Reference Strength, σ_0	1.45 GPa	~3 GPa	~4 GPa
Weibull Modulus, m	7.5	3.9 – 5.7	3 – 6

3.2 Structural Design

The mechanical strength data obtained using planar and radiused hub flexure specimens can be used to provide design allowables for structural design. Standard finite element techniques were used to obtain stress distributions in the rotor. For much of the rotor design axi-symmetric models were utilized. For detailed design of blade roots and other features, three-dimensional global-local models were utilized. Figure 6 shows a stress contours from a global model and the local detail of a turbine blade trailing edge. The stochastic properties of silicon were introduced into the design using the probabilistic design code CARES [5] which applies the experimentally-determined Weibull probability density function at the integration points of the finite element model. This process allows for an assessment of the structural failure probability of the whole rotor. Results from such analysis can be presented graphically to allow design trades to be conducted. Figure 7 shows an example in which the effect of material reference strength and blade height on the failure probability are compared. As a practical matter, true probabilistic design is rather unwieldy, so design was usually conducted to an allowable stress (typically 1 GPa) and then the failure probability was calculated to check the estimated reliability. It should also be noted that given the very low toughness of silicon the failure probabilities can be heavily influenced by the introduction of flaws during processing and handling. This demands a conservative design approach and great care during fabrication.

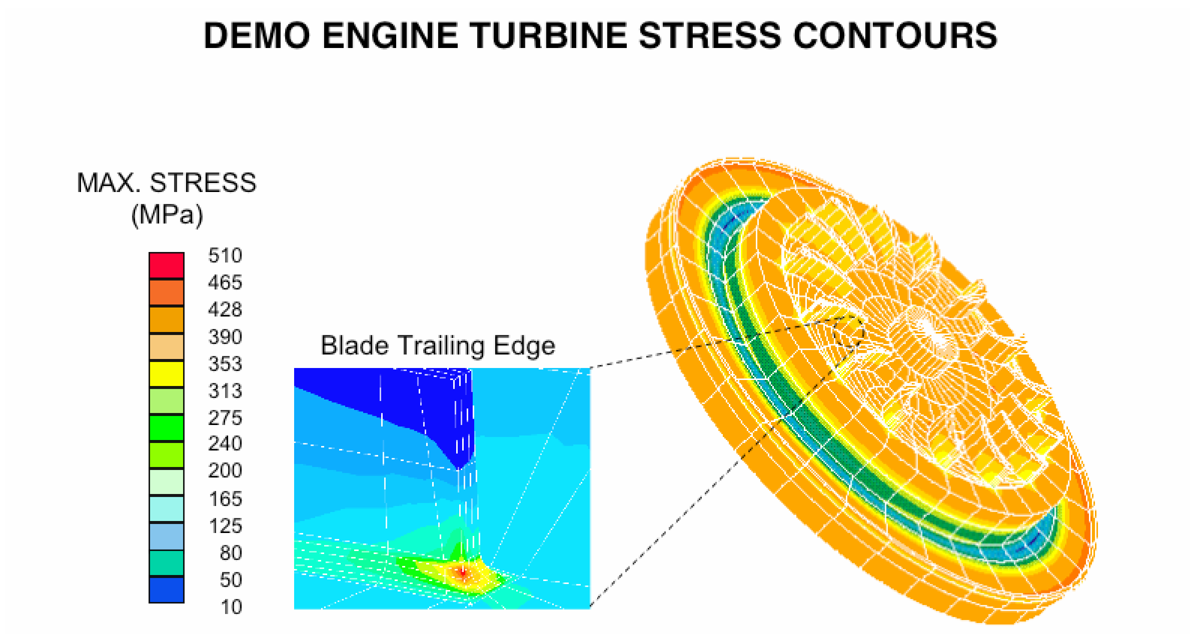

Figure 6: Turbine Stress Contours Obtained by Finite Element Analysis.

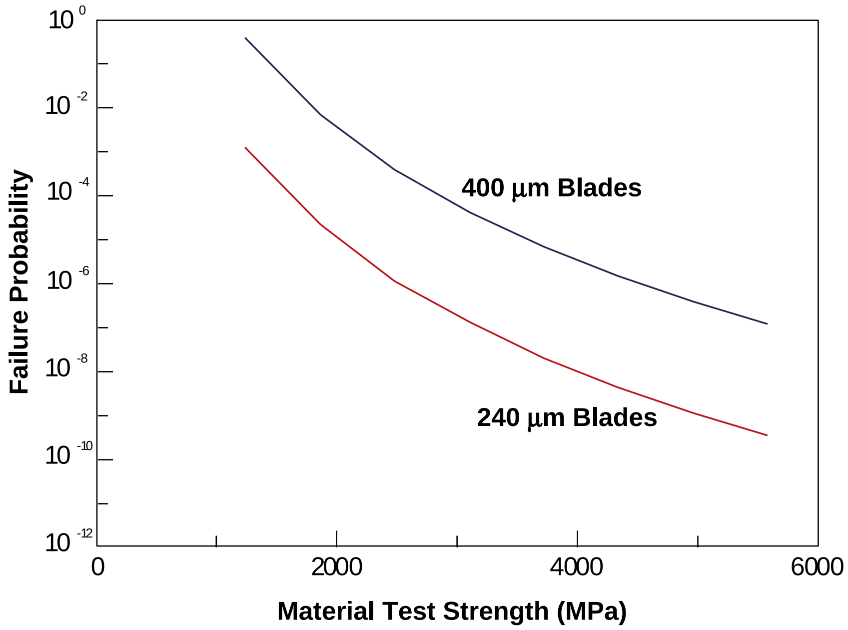

Figure 7: Failure Probabilities as a Function of Blade Height and Material Test Strength.

4.0 DESIGN FOR HIGH TEMPERATURE STRENGTH

Given the requirement for high temperature operation of the turbine spool, design for high temperature strength is of paramount importance. Silicon is not widely used at elevated temperatures, however it has attracted some attention as a model system for experiments to understand the fundamentals of plasticity. Figure 8 shows literature data for the elevated temperature response of silicon. The pronounced reduction in strength at temperatures above 550°C and the highly-non linear stress-strain response are of particular concern. Previous experiments [6] have shown that there is a tendency for damage localization due to slip band formation, as shown in figure 9 and 10 for four point bend specimens. In order to better understand the implications of this material behavior for structural design a constitutive model has been developed.

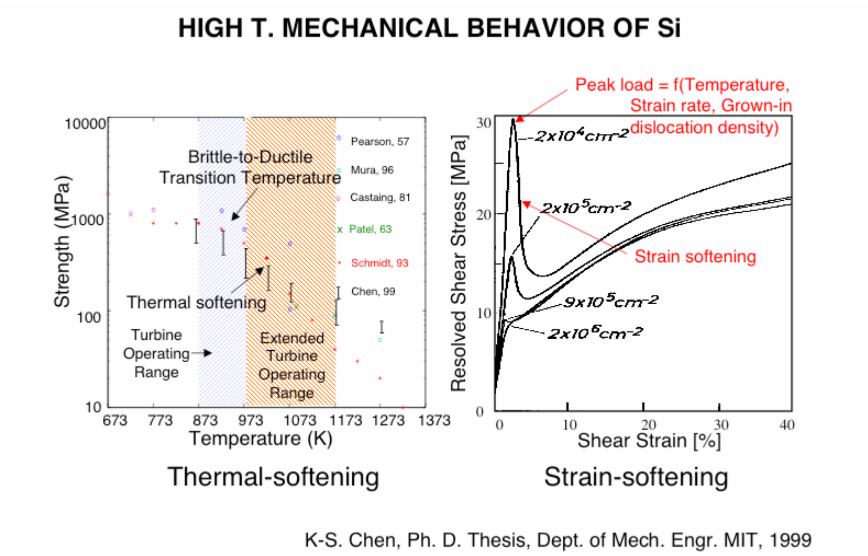

Figure 8: High Temperature Response of Si: a) Thermal Softening and b) Strain Softening.

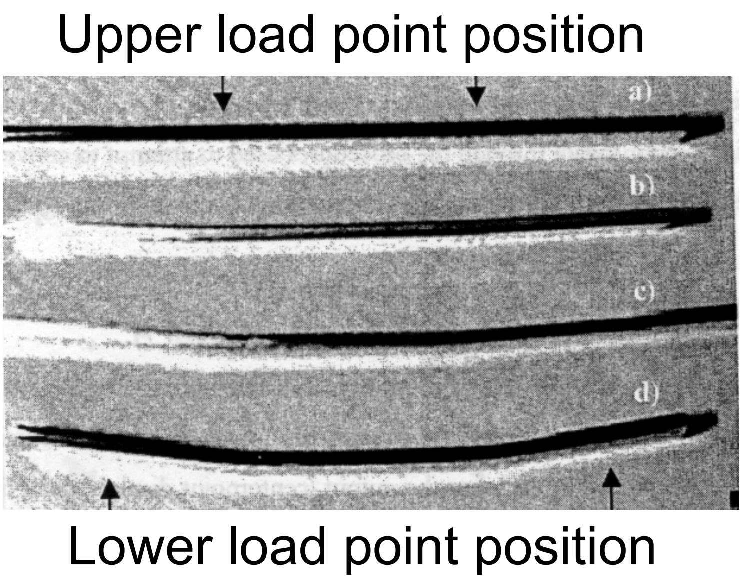

Figure 9: Si Four Point Bend Specimens Tested at Elevated Temperature. Note the pronounced deformation localization at the inner loading points.

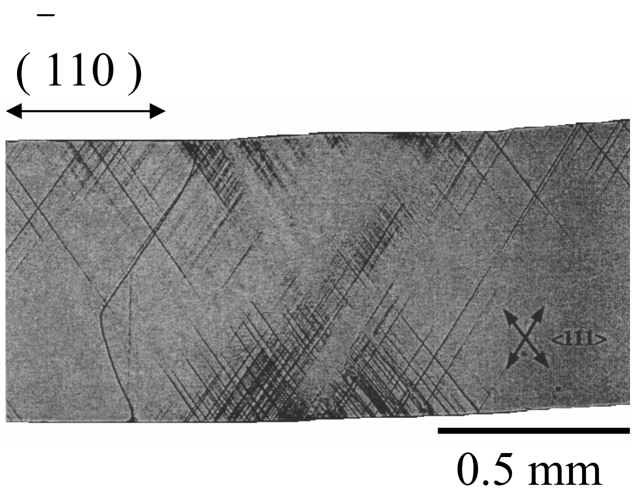

Figure 10: Polished and Etched Cross-Section of Region under the Inner Loading Points in Figure 9 showing High Concentration of Slip Bands.

4.1 High Temperature Material Model for Si

The material model was based on an existing isotropic plasticity model developed for metals. Two deformation mechanisms regimes are accounted for. At low dislocation densities, dislocation nucleation is the rate determining mechanisms. At high dislocation densities dislocation interactions control deformation. Two internal state variables, the dislocation density and the internal shear resistance are used to characterize the material. Evolution equations are expressed in terms of stresses, strains and temperature. The model is largely empirical, requiring 15 parameters to be calibrated. However, the physical basis of the internal state variables ensures that there is some predictive capability. A complete description of the model is beyond the scope of this lecture, but can found elsewhere [7, 8].

The model is calibrated by uniaxial creep experiments using data such as that shown in figure 11. Data was obtained from uniaxial compression tests conducted at two temperatures (600°C and 800°C) and four stress levels at each temperature.

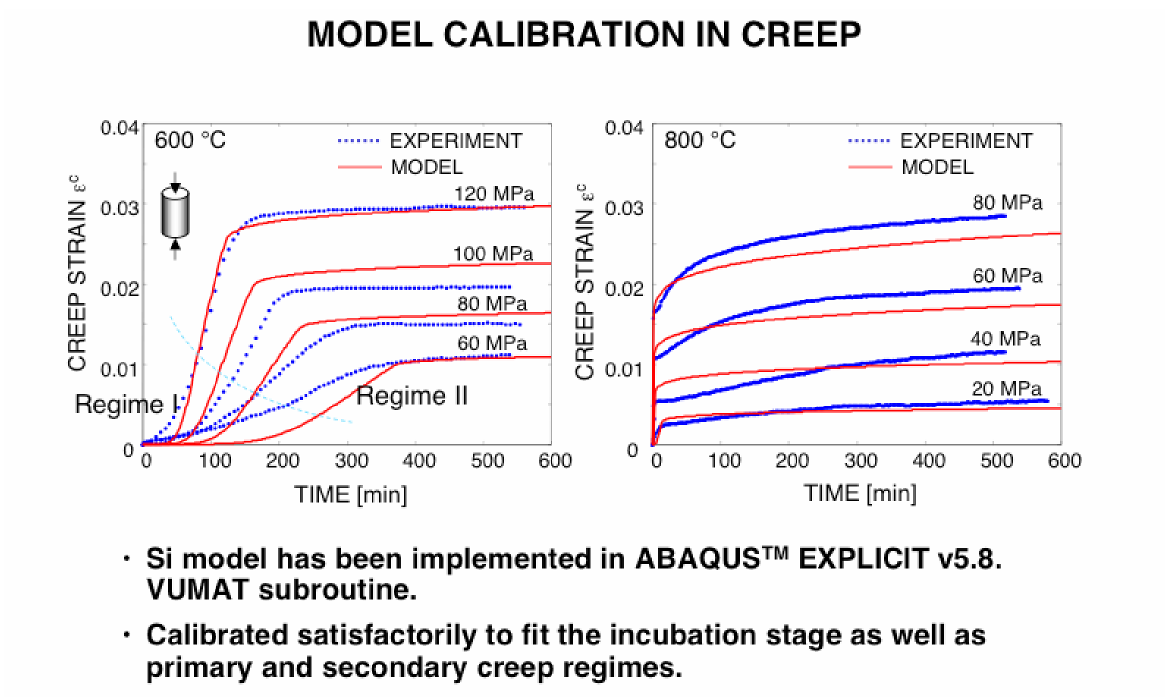

Figure 11: Uniaxial Creep Data for Silicon used to Calibrate the Constitutive Model.

Once calibrated the model was validated by using it to predict the response of the monotonic loading of four point bend tests. Data for specimens tested at three temperatures and two loading rates are shown in figure 12. The model provides a reasonable description of the data, thus confirming its validity for use in the structural design process. It is interesting to note that the relatively compliant four point bend specimen reveals pronounced strain softening behaviour, even though this is not directly evident from the stiffer, uniaxial compression creep tests shown in figure 11.

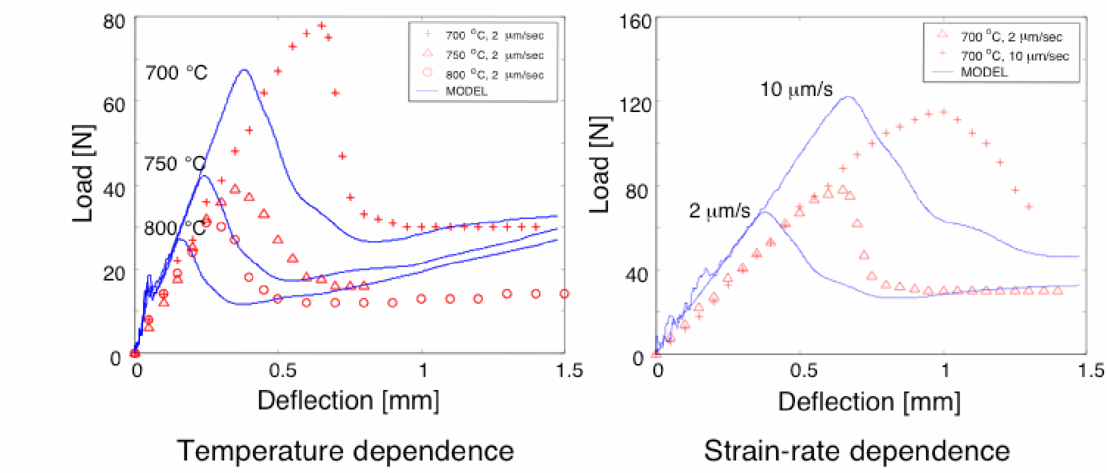

Figure 12: Model Predictions compared with Four Point Bend Data for Single Crystal Silicon.

Figure 13 shows data for four point bend tests in which the loading was interrupted and either a constant displacement hold or a constant load hold were applied. It is clear that for both cases the peak load achieved is reduced below that found in constant rate loading. This illustrates the issues of load history and the requirement for a conservative design approach if silicon is to be used as the structural material for a microengine.

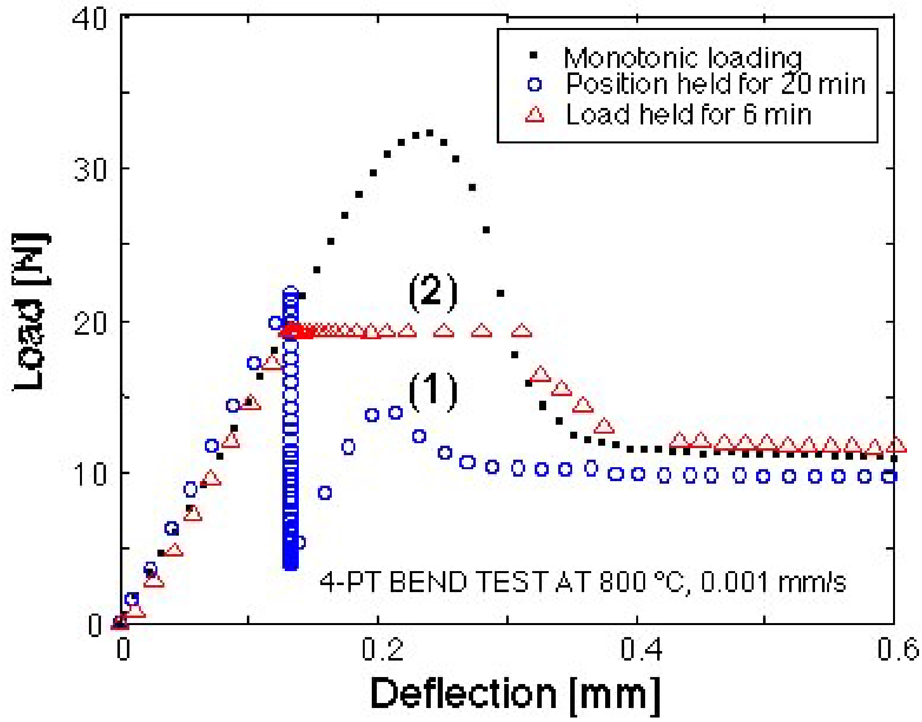

Figure 13: Experimental Results from (1) Strain Relaxation and (2) Hold at Load Tests Compared with the Monotonic Loading Case for Silicon Specimens in Four Point Bending.

5.0 USE OF SILICON CARBIDE IN HYBRID STRUCTURES

Given the temperature restrictions of silicon it is apparent that it is not an ideal material with which to construct high performance microturbomachinery. However, it is important to understand why higher temperature materials are required. In the MIT microengine design, the key limitation on the performance is not the material temperature directly, rather the heat conduction between the turbine and the compressor. The overall engine efficiency is significantly reduced by the large heat flux from the turbine to the compressor. If thermal insulation can be incorporated between the turbine and the compressor, then higher efficiency will be achieved. However, this requires that the turbine operate at a higher temperature than silicon allows. To this end more refractory materials have been assessed for use.

5.1 Mechanical Considerations in SiC/Si Hybrid Structures

The tolerances on the design of the bearings, in terms of defining the rotating gap and the mass balance of the turbine/compressor spool place significant fabrication limitations on the material options available. Essentially, they stretch the limits of conventional microfabrication capabilities, and significantly exceed those achievable in more conventional machining, moulding or casting processes. This implies the continued use of lithographic patterning and etching or deposition processes. However, the candidate materials, chiefly refractory ceramics are not generally amenable to such processes. Etch rates are low, and the degree of anisotropy and control that can be achieved are very limited. With this background a hybrid approach has been pursued that will allow the continued use of silicon microfabrication, but will provide structural reinforcement using silicon carbide. A detailed description of this approach can be found in reference [8]. Figure 14 shows a schematic of a microengine spool containing local silicon carbide reinforcement. Figure 15 shows finite element results which illustrate the structural reinforcement concept. The silicon carbide is much higher stiffness (460 GPa Young's modulus vs. 165 GPa for silicon) and retains its strength to temperatures in excess of 1600K. This means that the silicon carbide core of the spool carries the majority of the centrifugal load of the spool. Figure 16 shows the effect on the turbine material temperature of including 30% through the thickness of silicon carbide. Operation up to 1150K is achievable, which has a significant effect on overall engine efficiency, as it can cut the heat flux from the turbine to the compressor to ~5% of the all silicon case.

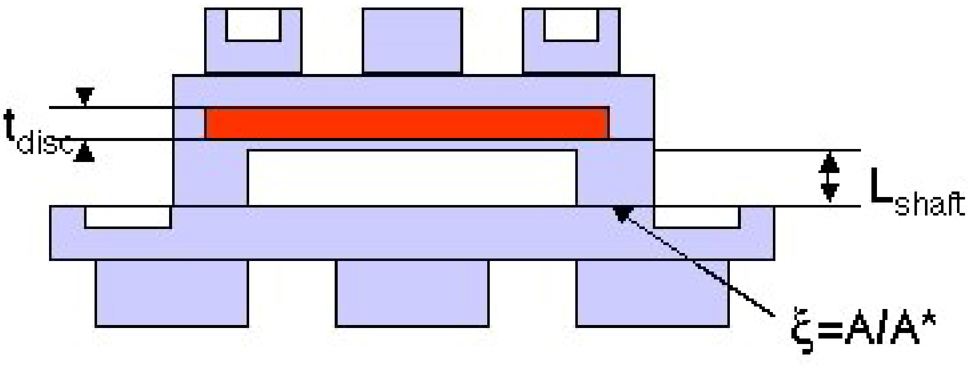

Figure 14: Schematic of Hybrid Structure Concept in which a Silicon Spool is Reinforced with Silicon Carbide.

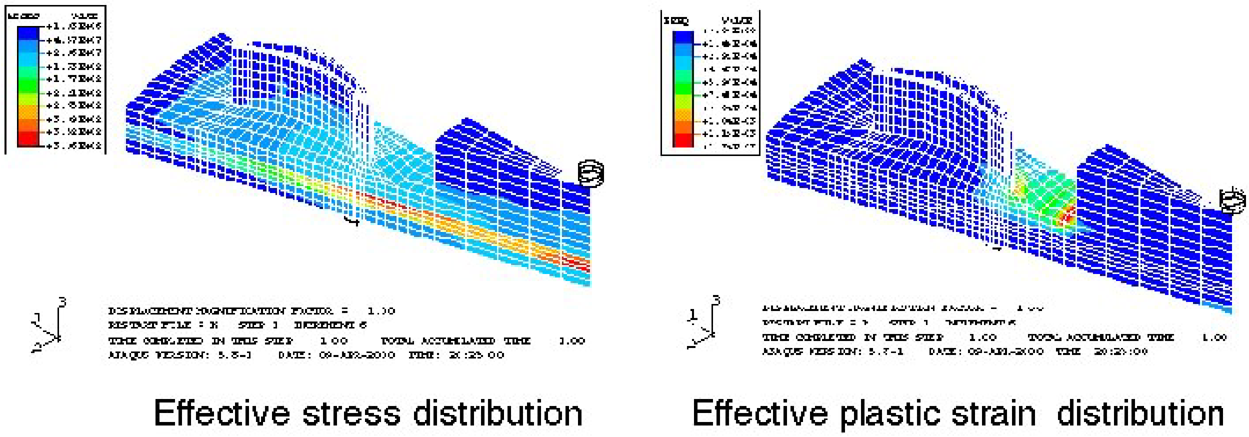

Figure 15: Finite Element Stress Contours and Plastic Strain Contours Showing the Reduction in Plastic Strain Resulting from the Incorporation of Silicon Carbide.

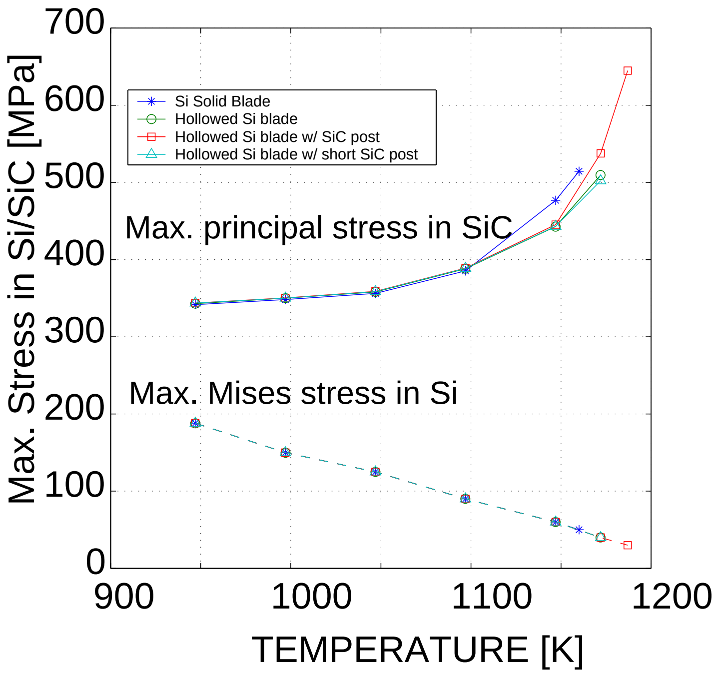

Figure 16: Illustration of Increased Operating Temperature Arising from Incorporation of Silicon Carbide.

5.2 Process Considerations in SiC/Si Hybrid Structures

The use of silicon carbide reinforcement can be achieved with relative simple processes that are compatible with the silicon microfabrication used for the first generation microengines. These are illustrated in figure 17. There are four key steps. (1) a circular pit is etched in a silicon wafer. (2) the pit is filled with chemical vapour deposited silicon carbide. (3) the overburden of excess SiC is removed by grinding and polishing and (4) a second silicon wafer is bonded over the Si/SiC surface of the first wafer. The bonded wafer pair moves through the rest of the process flow as though it were a monolithic silicon wafer. All the key dimensions (blades, bearings) are defined by silicon etching, which is well understood and can be controlled to the necessary tolerances. The details of the processes required will be the subject of the second lecture in this series.

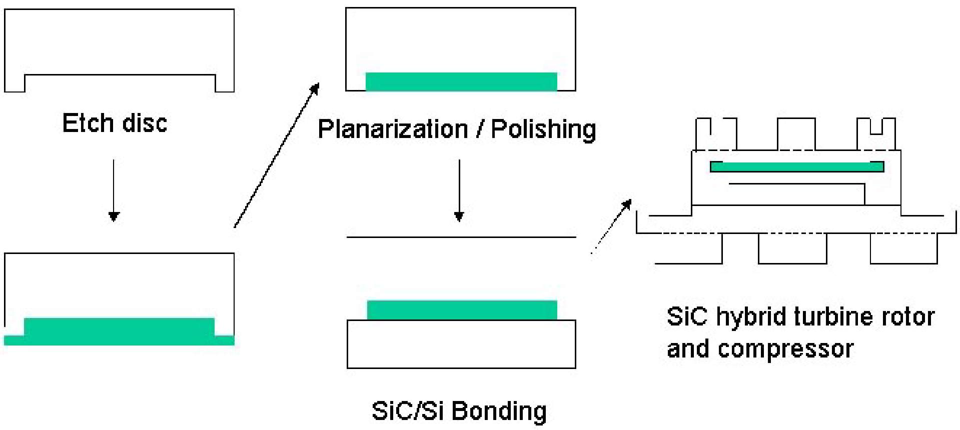

Figure 17: Schematic Process Flow for Creation of a Si/SiC Hybrid Spool.

5.3 Mechanical Test Results

The concept of Si/SiC structures has been partially verified by testing Si/SiC beams in four point bending. Results are shown in figure 18 and 19. The specimens were created simply by depositing SiC on Si and cutting them to size with a die saw. The specimens were then loaded in four point bending. Figure 18 shows results for different SiC layer thicknesses. Figure 19 shows that strength is retained at temperatures as high as 900°C (1173 K) as predicted by the FE model shown in figure 16. FE predictions are superimposed on the data in figure 19, further validating the Si Constitutive law. The SiC is assumed to be elastic with mechanical properties determined by micromechanical testing.

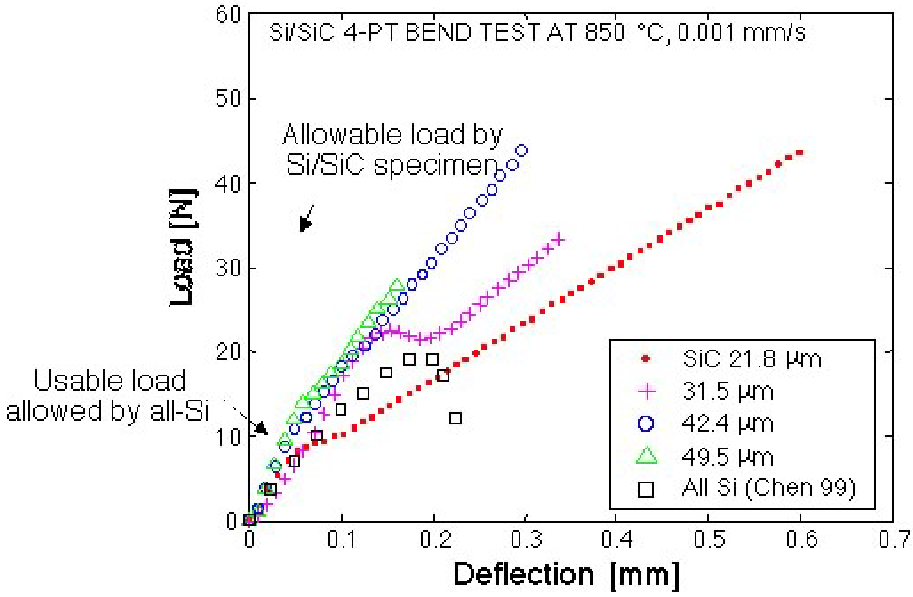

Figure 18: Mechanical Test Results for Si/SiC Hybrid Beams in Four Point Bending.

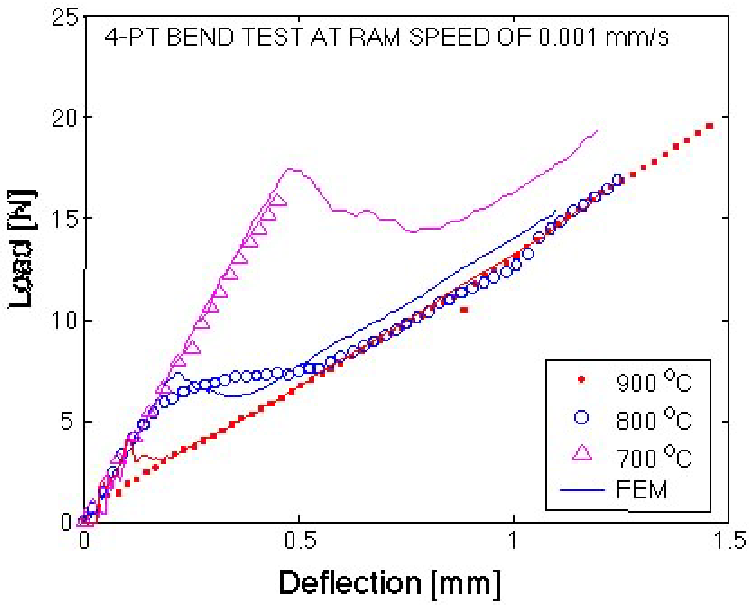

Figure 19: Four Point Bend Test Data and Model Predictions for Si/SiC Beams Tested at Three Temperatures.

Having validated the concept and the modelling, the model has been used to guide trades in the design of actual microengine rotors. Figure 20 shows a trades between maintaining a stable bearing operation (by mimizing reduction of the journal bearing air gap) with variations in SiC thickness and strength. Such trades help guide the effective determinination the division of program resources between material and process development and advanced bearing concepts.

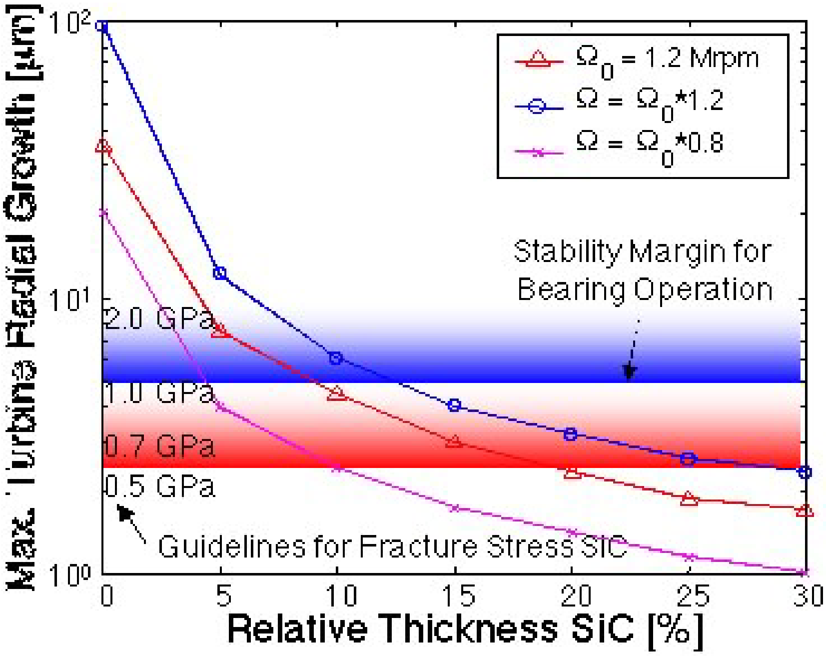

Figure 20: Tradeoffs in the Use of Si/SiC Hybrid Structures.

6.0 SUMMARY

This lecture has provided an overview of material selection and structural design issues associated with the MIT microengine concept. Key concepts covered have been:

1) The use of Weibull statistics and micro-mechanical testing to provide design guidance for low temperature structures.
2) The development of a high temperature constitutive model for Si, and its validation against material test data.
3) The use of Si/SiC hybrid structures in order to increase the allowable operating temperatures while minimizing the deviation from Si processes.

The following lecture will address key process technologies used in the course of the MIT microengine project.

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