Friction and Wear of Materials: Principles and Case Studies

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Lecture – 37
Computational Analysis in Assessing Wear

Hello, welcome back, so in this lecture, we would like to understand the significance of computational analysis in assessing the wear behaviour.

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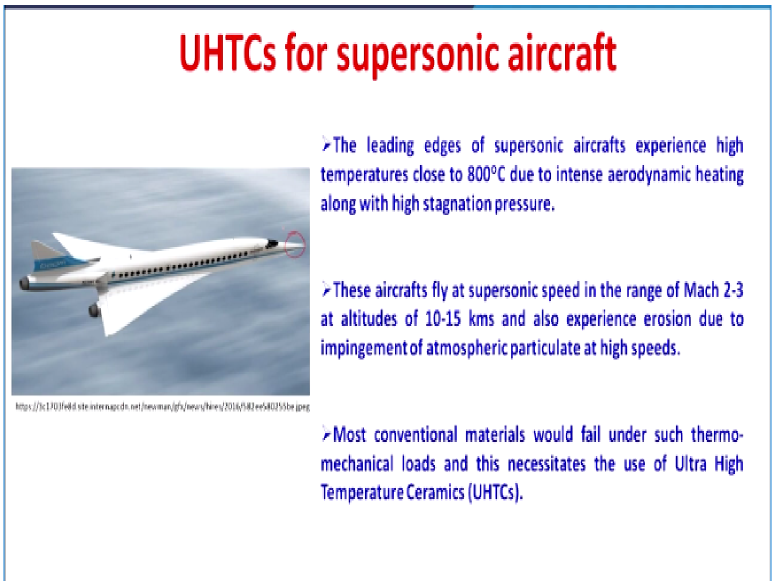

So, you might know that leading edges of supersonic aircrafts experience high temperature particularly at the nose edges or tailing edges and the temperature may rise around 800 Celsius as per the simulation studies, so this temperature rise is because of the intense aerodynamic heating along with the stagnation pressure. So, you know these supersonic aircrafts they travel at a very high speed of Mac 2 or Mac 3 at altitudes of around 10 to 20 kilometres.

And while travelling they may also experience erosion due to impingement of particulates those from the atmosphere and then these particle impingement may lead to the material damage, so most of the conventional materials they would fail under these thermo mechanical loads, so that necessitates the use of ceramics and the ceramics for this particular use that they have high melting points, so that you can use safely at these temperatures of 800,000 Celsius without any degradation in the strength.

Those ceramics are generally called ultra-high temperature ceramics, so ultra-high temperature ceramics are preferred for these components used for the supersonic aircraft, so in the family of the ultra-high temperature ceramics, zirconium di boride based ceramics are attractive because of their important properties.

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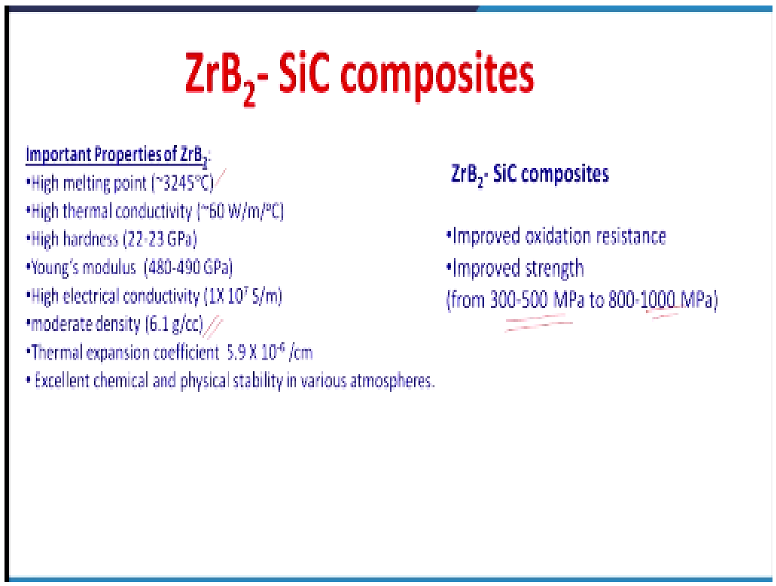

For example, very high melting point of more than 3200 Celsius and high thermal conductivity of around 60 watt per metre per Celsius, very high hardness, so that may lead to superior wear resistance, Young's modulus very high around 500 gigapascal and good conductivity and moderate density, this density; this moderate density is helpful for using this material for structural applications.

And so excellent chemical and physical stability in various atmospheres, those are candidate materials for a high temperature applications and it is already drafted in several reports that by adding certain amount of silicon carbide in zirconium di boride, we can improve the oxidation resistance of the ceramics and also you we can improve the strength of this ceramic, so for example without having silicon carbide, the zirconium di boride will have around 300 to 500 mpa strength.

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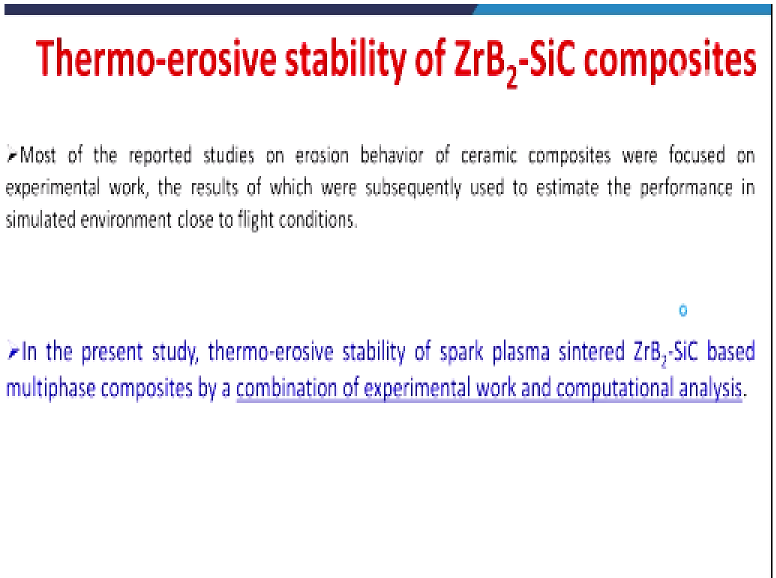

By adding silicon carbide, the strength may go even up to 1000 mpa, so but most of the reported studies and the erosion wear behaviour of ceramic composites, various ceramic composites not only zirconium di boride, whereas ceramic composites, they were focused on the experimental work and the results of this experimental work were subsequently used to estimate the performance in simulated environment.

And simulation studies, those simulated environments were selected which are close to the flight conditions that means, experimental work is done, the results of the experimental erosion work will be taken as input for the computational studies or the simulation studies close to the flight conditions now, in the present study we demonstrate a combination of the experimental one and computational work is more useful to understand the behaviour of these ceramic composites in high temperature erosion conditions.

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Computational analysis in understanding the experimental erosion test results on thermo-erosive stability of ZrB_2-SiC based composites

Particularly, we will see how this computational analysis will be helpful to understand that the erosion behaviour on erosion behaviour of zirconium di boride, silicon carbide based composites particularly, we will see the significance of computational analysis in understanding the experimental erosion test results on thermo erosive stability of zirconium di boride silicon carbide based composites.

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Objectives of the study

- To study erosion wear behaviour of the ZrB_2-SiC-Ti composites using a solid particle erosion tester at high temperature (800°C)
- To elucidate dominant mechanisms of material removal in wear conditions
- To determine the spatial temperature and stress distribution in the eroded region using finite element (FE) analysis
- To understand on the thermo-erosive-structural stability of ZrB_2-SiC-Ti composites

So, the objectives of the present study are to study the erosion behaviour of zirconium di boride, silicon carbide and titanium composites using a solid particle erosion tester at high temperatures of 800 Celsius and to understand the dominant wear mechanisms in the selected erosion conditions and mainly to determine the temperature and stress distribution in the eroded region using finite element analysis and to understand finally, the thermo erosive structural stability of the selected zirconium di boride silicon carbide titanium composites.

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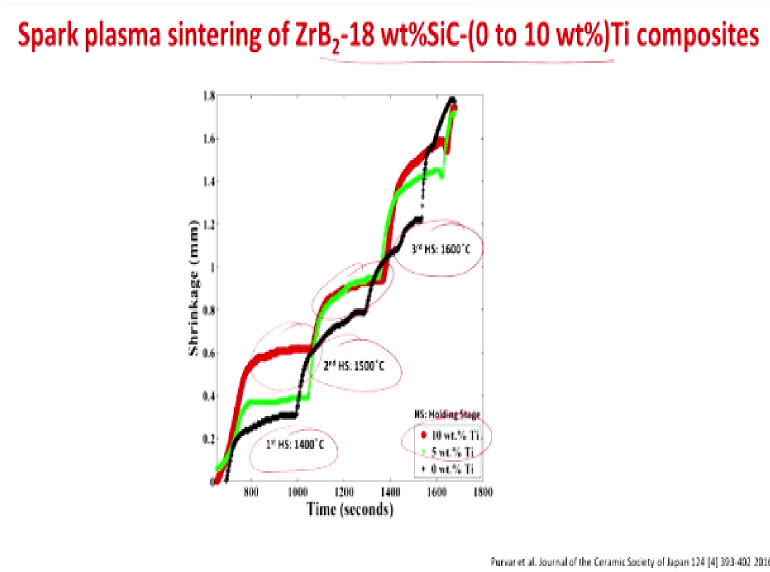

So, these composites were prepared by spark plasma sintering, first the powders of the zirconium di boride, silicon carbide and titanium were taken and mixed in a proportion of zirconium di boride with 18 weight percent of silicon carbide with the titanium amount varying from 0 to 10 weight percent, so these powder mixtures were kept in a dye and then subjected to spark plasma sintering.

So, spark plasma sintering gave a decent density of more than 98% density, so we can see the spark plasma sintering result the shrinkage versus time in this particular experiment, the spark plasma sintering was done in a 3 stage process, this is called multistage spark plasma sintering, so based on the previous understanding, so multi stage spark plasma sintering was conducted, so we can see at 1400, there was a holding of 5 minutes and then at 1500, there was a holding of 5 minutes and finally 1600 there was a holding of 5 minutes.

So, this shrinkage versus time curve for different composites are shown, now in general we can see there are 3 stages of the shrinkage increase corresponding to the sintering stages, so first the in general, the rate of the shrinkage is lower in first stage and a bit higher in the second stage and aggressively; the very aggressive shrinkage rate is aggressive in the third stage, with respect to composition, now you can see when the titanium was used.

So, we can see shrinkage was higher in particularly, the first and second stages, so this helps us so, this indicates the addition of titanium in the composite powder mixture of zirconium di boride and silicon carbide will improve the densification or will density material at lower stages of sintering itself so, the shrinkage further increase it to the next stage and then maximum shrinkage was obtained in the third stage of sintering.

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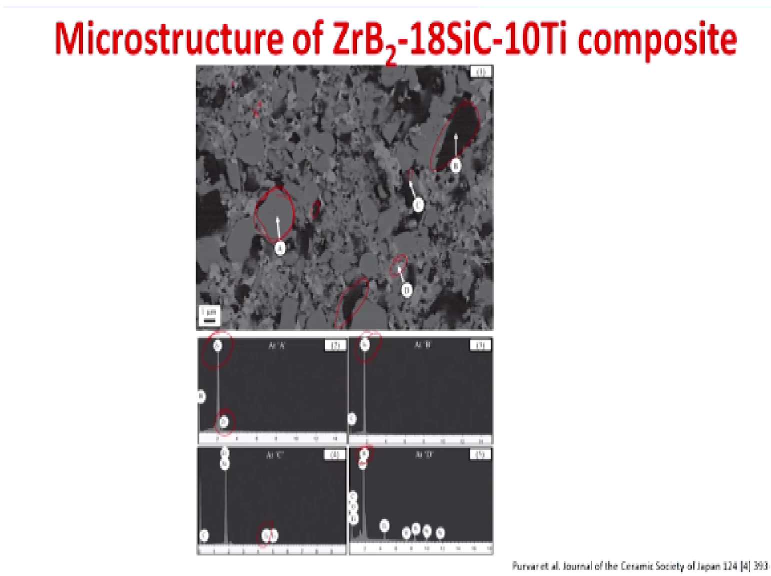

The microstructure of these composites particularly show zirconium di boride grains and silicon carbide particles, right, silicon carbide particles and then titanium, so the titanium being a lower melting material, so it forms a liquid melt while increasing the temperature during sintering, so this liquid melt penetrates between the particles of the zirconium di boride and silicon carbide and facilitates sintering.

So, such a liquid phase sintering gives us a densification earlier than that used without this titanium, so this zirconium di boride silicon carbide or particles of zirconium di boride grains and the silicon carbide particles are distributed and then we can see the EDS analysis of these particular phases, this A phase, this is zirconium di boride that is you can see significantly, the zirconium and boron, so zirconium di boride and you can see this black phase or darker phase which is rich with the silicon.

So, this silicon carbide and silicon carbide and we can see the zirconium and silicon both are present along with the titanium in the matrix and we can also see certain contamination from the ball milling medium, so ball milling was done mainly to mix these borders of zirconium di boride, silicon carbide and titanium, so but the ball milling was done by using balls of tungsten carbide.

So, tungsten carbide came into the powder mixture, so it still remains so, you have a contamination even after the sintering, so zirconium di boride grains and silicon carbide particles so, in this matrix of zirconium di boride grains and silicon carbide particles, we have certain zirconium silicon titanium rich phase in a different; at different locations.

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Mechanical properties of composites

Composition	Designation	Hardness (GPa)	Fracture toughness $MPa.m^{1/2}$
ZrB_2-18wt %SiC	ZST0	17.5±0.9	3.7±0.7
ZrB_2-18 wt% SiC-10%Ti	ZST10	29.2±2.0	9.0±0.9

Purvar et al. Journal of the Ceramic Society of Japan 124 [4] 393-402 2016

So, these 2 materials of zirconium di boride with 18% silicon carbide and zirconium di boride with 18% silicon carbide and 10% silicon carbide were taken for investigating the erosion wear behaviour so, these are designated as ZST0, ZST10. ZST0 means no titanium, T10 means 10% titanium, the hardness and the fracture toughness values were determined by Vickers indentation so, you can see the hardness increased from 17.5 gigapascal to around 29.2 gigapascal by adding 10% titanium in the baseline composition zirconium di boride silicon carbide.

And fracture toughness also improved from 3.7 to 9.0 mpa root meter, so you see there is very large improvement in the hardness and fracture toughness by adding only smaller amount of 10% titanium in the composite, so it also indicates the densification is improved by adding a titanium that reflects in the microstructural characteristics and then the mechanical properties so, in another study it was also found that the grain size of the zirconium di boride or particle size of silicon carbide are almost similar to that what we started as an initial powder particles.

So, there is no much difference in the size of; average particle size of silicon carbide or average grain size of the zirconium di boride, so this also indicates the spark plasma sintering conditions were sufficient to prepare a material of higher density with good mechanical properties, among the two investigated composites, the composite with the titanium showed higher hardness and fracture toughness.

Among the investigated composites, the composite with titanium addition showed higher fracture toughness and higher hardness, so with this information, so we conducted the high temperature erosion test, so high temperature erosion test was done using a high temperature particle erosion tester.

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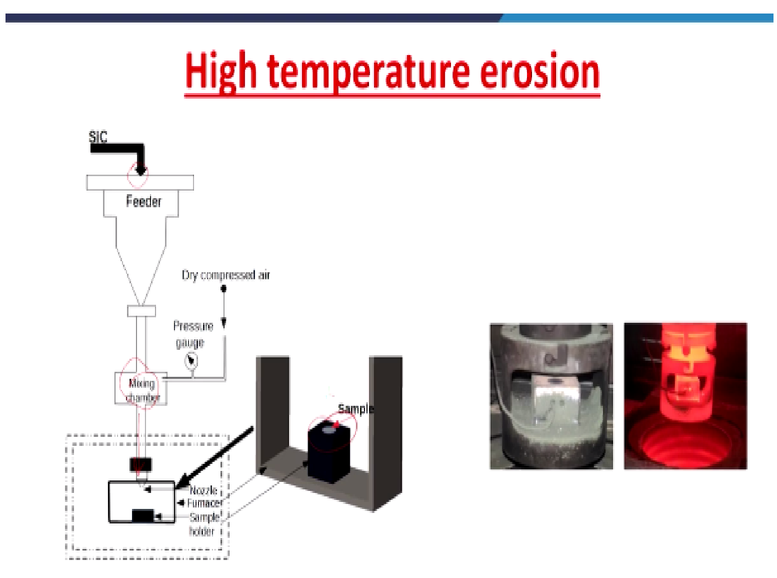

So, silicon carbon particles which we called erodent's of around 40 to 50 micron meter size; particle size were mixed with air and then the this mixture were used to erode the surface of the composite, so we can see the real time photograph of this material, when it was at a high temperature of around 800 Celsius, so we see this kinetic energy per unit area for the leading edge of the hypersonic vehicle flying at a Mac 10 speed at 30 kilometres altitude.

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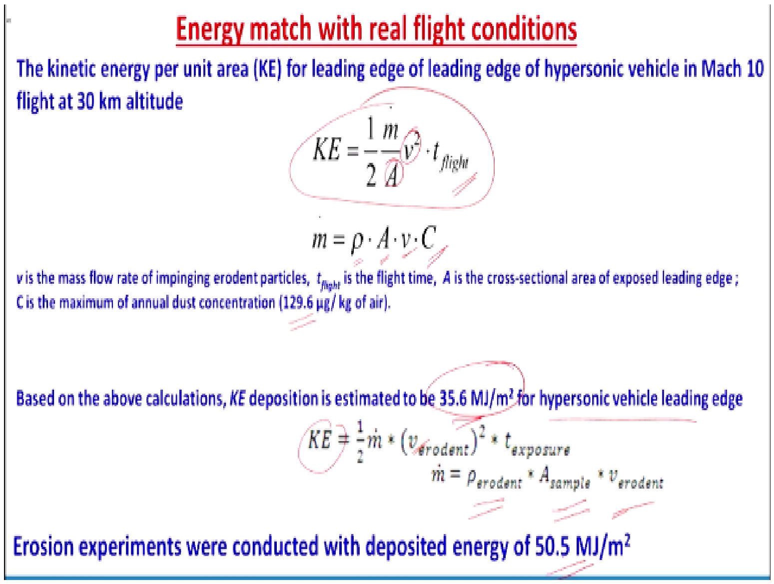

So, the kinetic energy can be estimated, if you know the flight time and the cross sectional area of the exposed leading edge and this mass flow rate of this impinging erodent particle, where this m dot can be found out by density area cross sectional area of the leading edge, the particle flow rate, mass flow rate of the particles and see a constant generally, max c is a maximum of annual dust concentration which was taken at 129.6 micron gram per kilogram of the air.

So, this was taken from the literature, okay, based on the above calculations, the kinetic energy deposition is estimated in for the hypersonic vehicle leading edges is around 35.6 mega joules per meter square, so the kinetic energy we know this by 1/2 m dot v square t of exposure, so we know the mass flow rate of the impinging particle, time of exposure in the test and then we know the density of this erodent, the sample cross sectional area.

The erosion experiments were conducted with the deposited energy of around 50.5 mega joules per meter square, a very higher more than 130% than what we have as a kinetic energy deposited so, just for the safe side and we took a further condition which give us the kinetic energetic position of around 50.5 mega joules per meter square.

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Erosion test parameters

Parameter	Value
Erodent particle size	>25 µm
Equivalent force	25 mN
Pazrticle velocity	47±1 m/s
Particle feed rate	3±0.2 g/min
Impact angle	90º
Time of testing	1200 s
Operating temperature	1073±100 K
Pressure	101.32 kPa
Energy deposited	50.5 MJ/m²

So, we selected the parameters accordingly and the particle size velocity and the time of testing was 1200 seconds and the erosion was done at 90 degrees impact angle, so we get around 50.5 mega joules per meter square, so the sample surface first exposed to equivalent heat deposition as given here.

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Erosion test

Sample surface was exposed to equivalent heat deposition

$$\dot{q}_e = \frac{1}{2} * \rho_{erodent} * A_{sample} * (v_{erodent})^3 * t_{exposure}$$

Force equivalent of momentum lost by erodent per unit time $F = \dot{m} * v_{erodent}$

Erosion experiments were done at 1073K and normal impact

And the force equivalent of momentum lost by erodent per unit time were also calculated, so but erosion experiments were done at 1073 kelvin that is 800 Celsius and normal impact, so this selection of these 1073 K is also based on the limitation of the erosion test equipment and normal impact was selected because we know the ceramic composites, they usually fracture to a larger extent at 90 degrees angle and then that lead; and lead to maximum wear. So, we selected these two; temperature and the angle.

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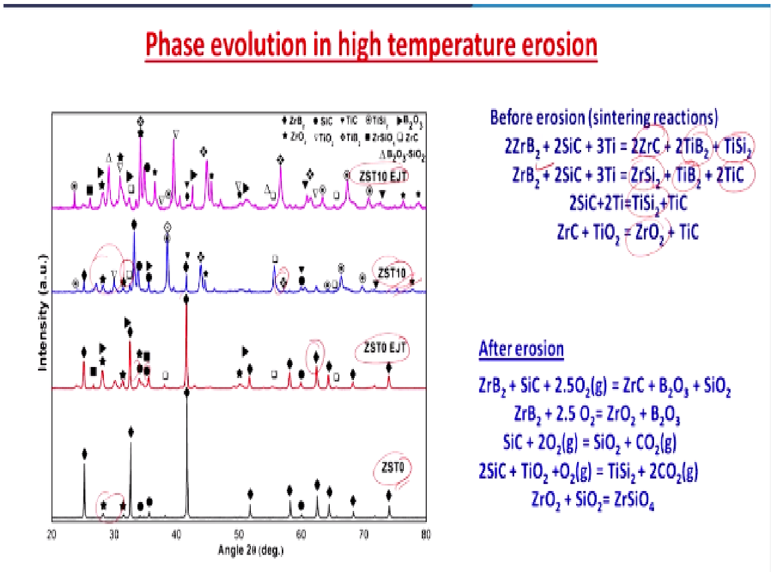

So, now we can see the x-ray diffraction analysis for understanding the phase evolution in high temperature erosion, so we know we see here this ZST0 means before erosion that is after sintering and ZST0 EJT means erosion tested similarly, ZST10 before erosion and ZST10 after erosion, now you see the phases before erosion or just zirconium di boride silicon carbide and zirconium oxide, right for the sample without having the titanium.

When titanium was added in the powder mixture on sintering was done, so the sintering reactions or that means before erosion, we have certain sintering reactions, zirconium di boride, silicon carbide with titanium that gives zirconium carbide titanium di boride and also zirconium silicide and titanium boride titanium carbide titanium silicide zirconium oxide, so several possible reactions can be thought.

So, after erosion, we still have few new phases formed on the surface, zirconium di boride silicon carbides, right and then along with this, we also have zirconium carbide, boron oxide, silicon oxide and then titanium silicide ore zirconium silicate, so there are certain new phase is formed because of the high temperature erosion, so let us understand such phase analysis by considering the thermo dynamics and the kinetics.

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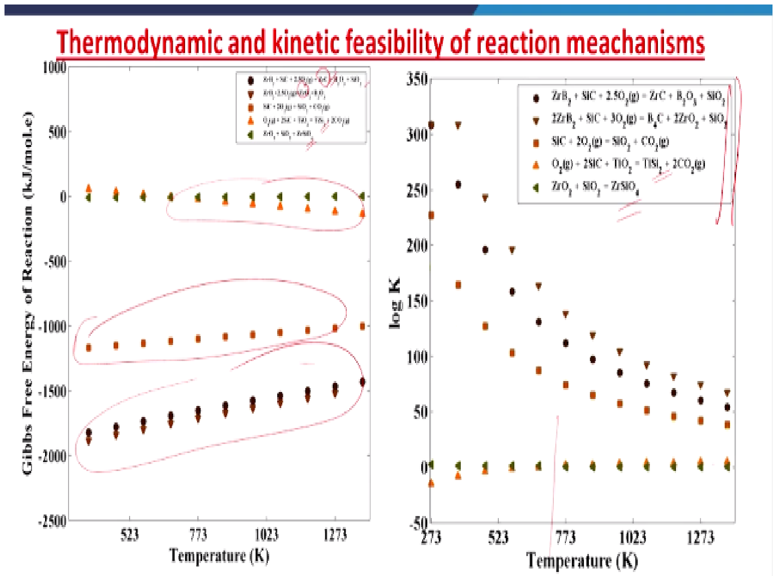

So, after sintering the erosion was done and that these are the probable reactions because we are seeings all this reaction products, so these reaction products are big thought to be because of the; these reactions, right, so let us understand the feasibility of such reaction mechanisms by thermodynamics or kinetics. So, Gibb's free energy versus temperature was plotted for these reactions, these reactions.

And we can see the formation of this zirconium carbide, we can see here the formation of the zirconium carbide, boron oxide or silicon oxide right, so we can see it is feasible within this temperature range of around this 500 to 1273 K within this range, these are largely negative that means, it is highly possible reaction forming a zirconium oxide, so similarly zirconium oxide and zirconium carbide.

So, silicon oxide of is usually formed on the silicon carbide surfaces and in the high temperature, so we still have this thermodynamically this is feasible whereas, the formation of titanium silicide and zirconium silicate, are also possible generally at more than 1000 Kelvin but these are still nearer to the 0 value of this Gibb's free energy, so we can say that these are still feasible, right.

And the equilibrium constant was also plotted as a function of time, you can see all reactions have the equilibrium constant positive that indicating the feasibility of such reactions and of course with the titanium silicide and zirconium silicate formation is generally possible at more than 1000 Kelvin right, so these reaction mechanisms are possible and this fact is supported by the thermodynamic and kinetic feasibility as well, right.

So, all these reactions are possible in the high temperature conditions used for the erosion, so we have certain zirconium carbide, boron oxide, silicon oxide, boron carbide, zirconium oxide, silicon oxide, titanium silicide, zirconium silicate etc., so we have several phases on the surface, right. One important observation is there is no titanium here, so even before starting the erosion just a sintering itself resulted into certain compounds of titanium boride, titanium silicide, titanium carbide.

So, we do not have any metal; metallic titanium, so that indicates that the titanium was consumed completely during sintering and then form different phases, right because of the formation of these hard phases, so we have an improvement in the hardness and fracture toughness.

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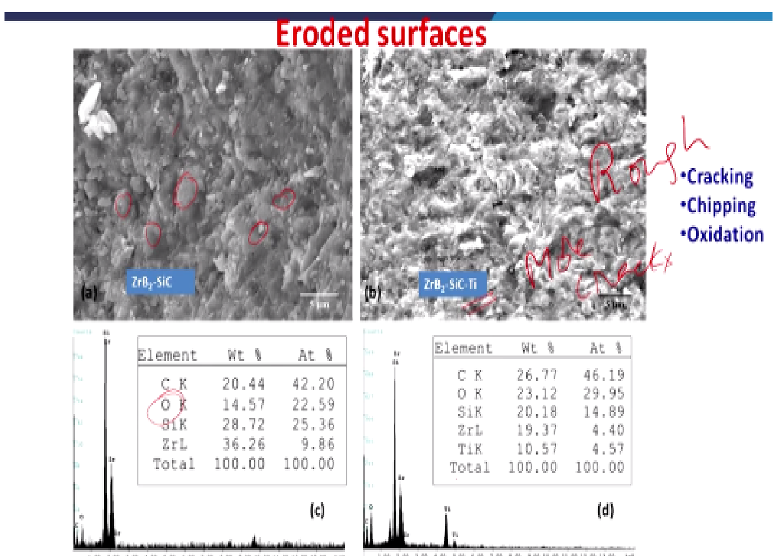

Element	Wt %	At %
C K	20.44	42.20
O K	14.57	22.59
SiK	28.72	25.36
ZrL	36.26	9.86
Total	100.00	100.00

Element	Wt %	At %
C K	26.77	46.19
O K	23.12	29.95
SiK	20.18	14.89
ZrL	19.37	4.40
TiK	10.57	4.57
Total	100.00	100.00

So, let us understand the mechanisms of the material removal in the given erosion conditions, so you see these zirconium di boride silicon carbide, there is lot of chipping and then the cracking, EDS analysis also indicates the oxidation, so when the titanium was added, you can still see the chipping and cracking even the surface becomes more rough, right more rough that means, it indicates more cracking, more cracks, right.

So, more cracking and chipping and the oxidation so are also are observed in the eroded material of zirconium di boride silicon carbide and titanium, so overall the material is removed by cracking, chipping and oxidation for these 2 composite materials.

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High temperature erosion test results

Designation	Volume loss per kg of erodent (mm^3/kg)	Hardness (GPa)	Fracture toughness $MPa.m^{1/2}$
ZST0	35.86±1.50	17.5±0.9	3.7±0.7
ZST10	33.49±0.09	29.2±2.0	9.0±0.9

A combination of 1.7 times increase in hardness and 2.5 times increase in fracture toughness (with 10% Ti addition in ZrB2-SiC) → 6.6% improvement in erosion wear resistance

The results from the high temperature erosion indicate so, the high temperature erosion test the material removed is measured by weight loss and converted into volume loss and then converted into volume loss per kilogram of erodent that we called erosion rate, so the high temperature erosion test results show that there is a decrease in the erosion rate from ZST0 to ZST10, you can see from 35.86 mm cube per kilogram to 33.49 mm cube per kilogram change in erosion rate observed when we add 10% of titanium in the composition.

And if you relate these; behave this erosion rate with the mechanical properties, we can see there is a large improvement in the hardness and fracture toughness, almost 1.7 times increase in the hardness and 2.5 times increase in the fracture toughness by adding 10% of titanium in the baseline zirconium di boride silicon carbide composite but this combination of increased mechanical properties resulted only 6% or 6.6% improvement in the erosion wear resistance.

So, there was a large improvement in the mechanical properties by adding 10% titanium in zirconium di boride silicon carbide composite but this reflected in only 6.6% improvement in the wear resistance, this is very interesting.

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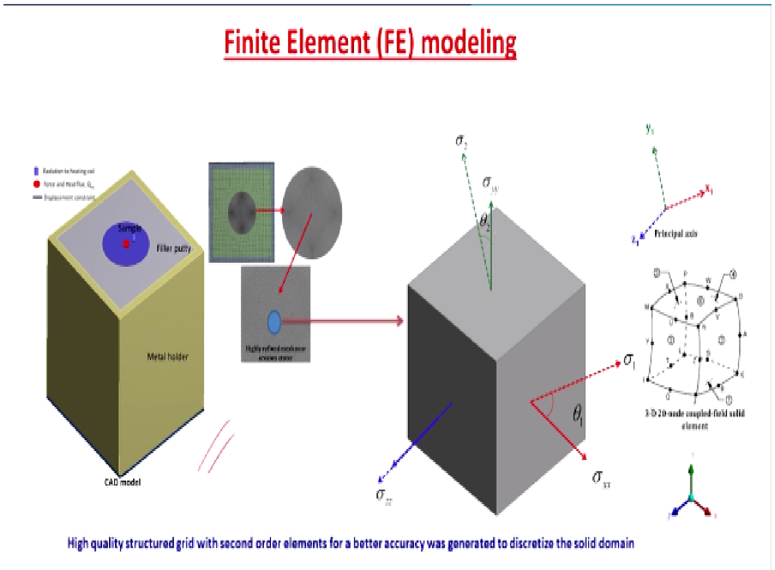

So, now this is where we need computational analysis to understand such a behaviour, so for this finite element modelling was carried out, right using ANSYS software, so you can see the CAD model high quality structured grid with second order elements for a better accuracy was generated to discretise the solid domain, we can see the CAD model here, this is the sample, right sample.

And then we can see the highly refined mesh near the erosion crater, so this can be explained by the three dimensional 20 node couple field solid elements, so these sigma indicates the principal stresses on each element, so all the properties like thermal conductivity.

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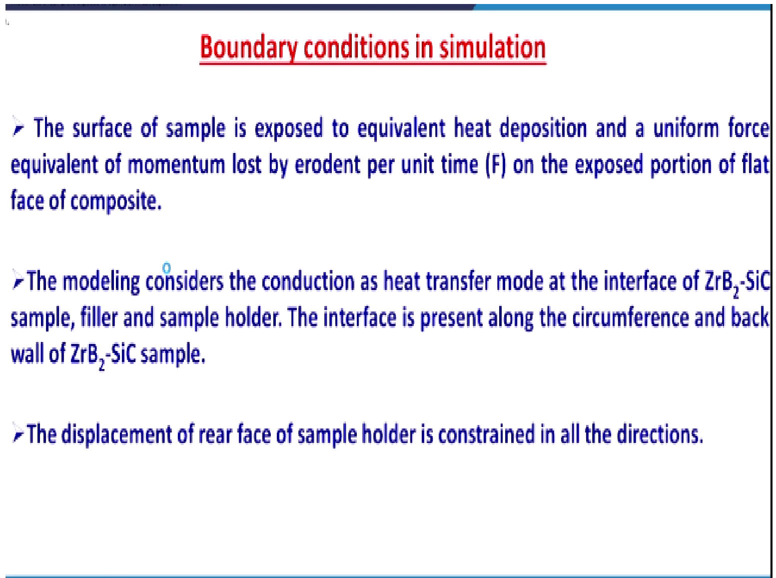

So, in the FE modelling, the boundary conditions used are the surface of the sample is exposure to equivalent heat deposition and a uniform force equivalent of momentum lost by the erodent per unit time and the exposed portion of flat face of the composite and other boundary condition is modelling; in modelling we consider the conduction as the heat transfer mode at the interface of this zirconium di boride silicon carbide sample, filler and sample holder.

So, we have this filler; filler is used to fix to the sample inside this metal holder, sample holder, the interface is present along the circumference and back wall of the zirconium di boride silicon carbide sample, so we know this; we have the displacement constraints even at the back wall right and along this walls of the holder. The displacement of rear face of the sample holder is constrained in all the directions, right.

So, stress and the temperature distribution were studied first by transient thermal analysis and then thermo structural analysis.

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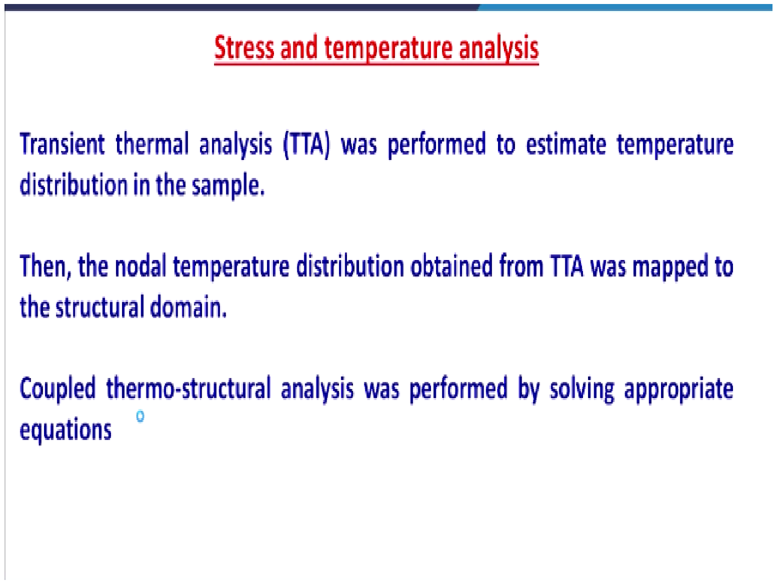

First initially, transient thermal analysis was performed to estimate the temperature distribution in the sample, then the nodal temperature distribution obtained from the transient thermal analysis was mapped to the structural domain and then we have a coupled thermo structural analysis by solving appropriate equations, so first the results from the transient thermal analysis.

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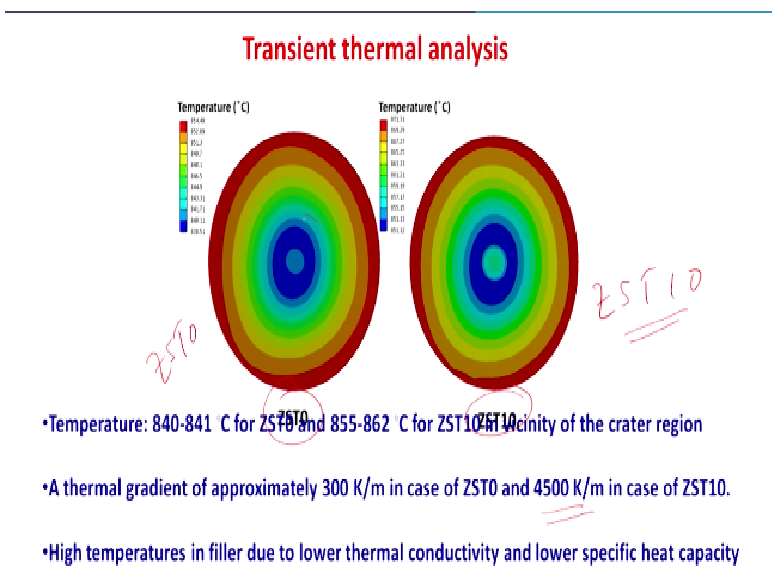

So, we can see this is a sample of ZST0, this is sample of ZS10, this is ZST10, this is ZST0, now you see the temperature distribution here, for the ZST0, the temperature interval you can see here for around 840 to 841 in the vicinity of this crater region whereas, for the ZST10, in the vicinity of the crater region, the temperature interval is between 855 to 86, so a thermal gradient of approximately 300 Kelvin per metre, in case of ZST0 and 4500 Kelvin per metre in case of ZST10 were observed.

So, high temperatures are also absorbed in the filler material and because mainly because of its lower thermal conductivity compared to these 2 samples either ZST0 or ZST10, compared to these two sample materials, the thermal conductivity or the filler material is very low, so the conduction is difficult in the region of this filler, so you get a high temperatures at the filler regions, this can also be due to lower specific heat capacity of the filler compared to these two materials.

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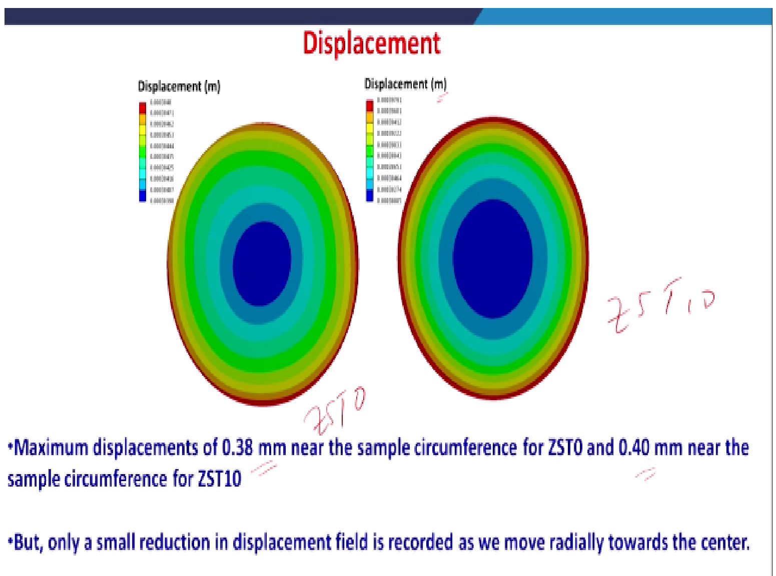

So, you can also see the displacement analysis, so the display; this is again, this is for ZST0, it is ZST10, right so, maximum displacement of around .38 mm near the sample circumference for the ZST0 and .40 for nearer; .40 mm nearer the sample circumference of ZST10 are found, right, you can see this is in meter, so but only a small reduction in the displacement field is regarded as we move radially towards the centre.

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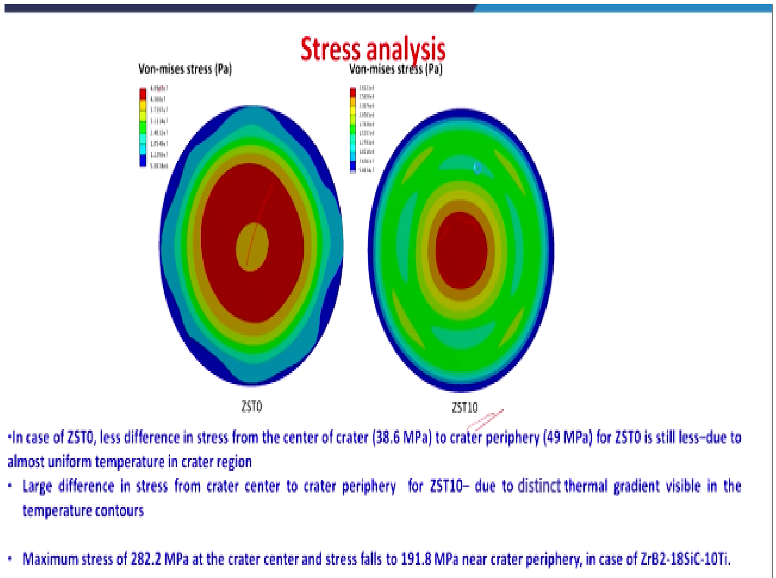

But if you see the stress analysis, so one my stress values were calculated, so in case of ZST0 there is a less difference in stress from the centre of this crater to the crater periphery, right to the crater periphery, so the stressors are around 38.6 mpa in the centre of the crater to 49 mpa for the crater periphery, you can see here 49 here, this is 10 power 7, so it is 38 to 49 mpa, if we move from the centre of the crater to the crater periphery.

So, this less difference in the stressors from the crater centre to the crater periphery for ZST0 is because of the less difference in the temperature in the crater region, so almost uniform temperature is maintained, so you do not have any difference in the stressors but if you see the ZST10, larger difference in stress from the crater; centre to the crater periphery, so this is mainly because of the distinct thermal gradient visible in the temperature contours.

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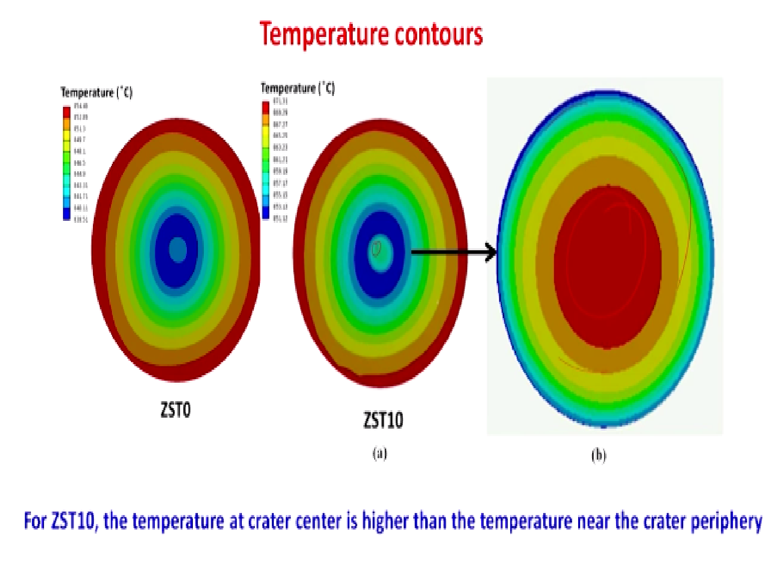

So, you can see there is a large difference in the temperature contours and you can see this centre of the crater is again nodded, so you can see for ZST10, the temperature at the crater centre is higher than the temperature near the crater periphery, so the stressors found were also very large in case of ZS10, so maximum stress of 282, you can see the maximum stress of 282 mpa is found at the crater centre and the and this is stress is; stress falls to 192 mpa nearer the crater periphery right, in case of this ZST10.

So, such a difference in the stressors can be understood because of the temperature differences from the centre of the crater to the periphery of the crater, so for this ZST10, the temperature at the centre is higher than the temperature at the crater periphery, right, we can see this crater, this is simulation for the temperature contours, this is the temperature contours for the crater region only.

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Stress analysis

- Inherent residual stress at room temperature due to differential coefficient of thermal expansion of various phases tend to relax at higher temperatures.
- Hence, stresses in oxidized sample as estimated in the present work using FE analysis are additional stresses developed during high temperature erosion.
- Less weight loss indicates the ability of the ZrB_2-SiC-based multiphase ceramics retain its properties in the stress conditions in high temperature erosion conditions

So, we must understand there are certain inherent stresses generated, so there are certain inherent residual stresses at room temperature because of the difference in coefficient of thermal expansion of various phases present in the material but these stresses tend to relax at higher temperature, so the stresses in the oxidised sample as estimated in this work using this finite element analysis or additional stresses developed during high temperature erosion.

So, we can also see there is very less weight loss because of this erosion, so this very less weight loss indicates the ability of this zirconium di boride silicon based multiphase ceramics to retain the properties in the stress conditions in the high temperature erosion, right.

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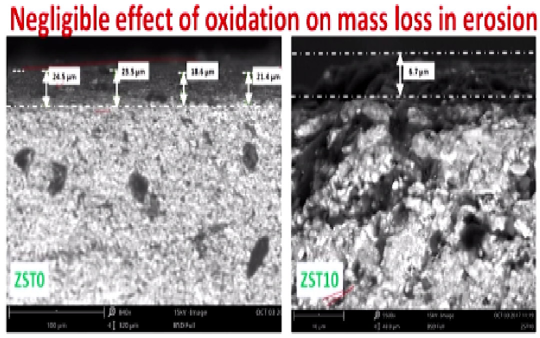
Negligible effect of oxidation on mass loss in erosion



Sample	Oxide layer thickness (μm)	Oxide layer mass (μg)	Mass loss due to erosion (g)	Ratio of mass gain due to oxidation to mass loss due to erosion
ZST10	6.7	5.99	0.17	0.0035
ZST0	25	22.45	0.18	0.0124

The additional presence of refractory compounds, TiC and $TiSi_2$ contribute in improving hardness /toughness of ZrB_2–18SiC–10Ti and leads to improved stability

Let us also understand the effect of oxidation on the mass loss in erosion very carefully, the samples were flattened to see the oxidation layer thickness, so this is ZST10, the maximum thickness of this oxide layer is around 25 micron meter, whereas for the ZST10, the maximum thickness is around 7 micron meter, you can see the ratio of mass gain due to oxidation to the mass loss due to erosion is very less, right.

So, .0035 for the ZST10 and ZST0 0.0124, so that means very negligible effect of the oxidation on the mass loss due to erosion, so the mass gain due to oxidation is negligible when you compared with the mass loss due to erosion that means, we can say the material is removed by the mass loss during erosion significantly, so we can also understand that the additional presence of the refractory compounds for example, titanium carbide titanium silicide, these contribute in improving the hardness or toughness for the zirconium di boride silicon carbide titanium composite.

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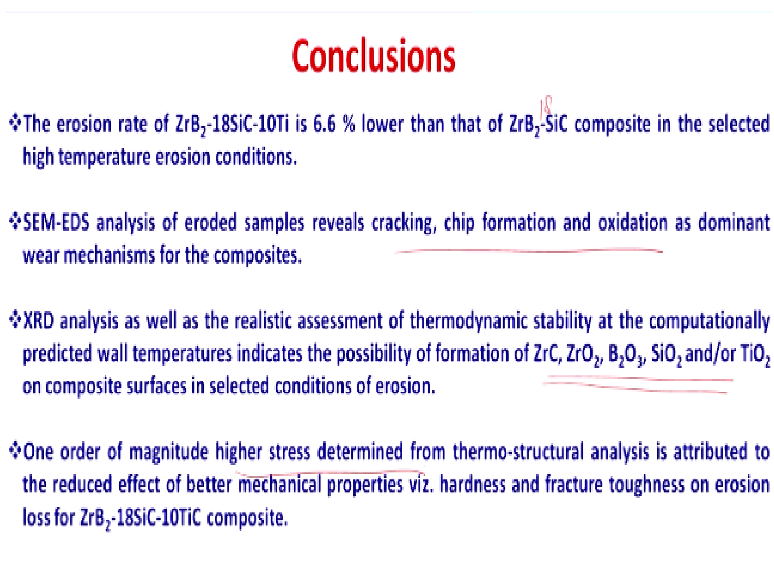

So, it leads to improved stability finally, let us conclude the salient results obtained from this study. The erosion rate of zirconium di boride silicon carbide titanium composite is 6.6% lower than that of zirconium di boride silicon carbide composite, this is also 18, the eroded samples reveals mainly the cracking, the chip formation and oxidation as dominant mechanisms of material removal for the composites.

X-ray diffraction analysis as well as the realistic assessment of the thermodynamic stability at the computationally predicted wall temperatures indicates the possibility of the formation of several phases, zirconium carbide, zirconium oxide, boron oxide, silicon oxide or titanium oxide on the composite surfaces in the selected conditions of erosion. One order of magnitude higher stresses are determined from the thermo structural analysis.

So, this higher stresses are attributed to reduced effect of better mechanical properties like hardness and fracture toughness and the erosion loss for the zirconium di boride silicon carbide titanium composite, so in spite of having large improvement in the hardness and fracture toughness, there was less improvement in the erosion wear resistance, for the zirconium di boride silicon carbide titanium composite compared to zirconium di boride silicon carbide.

So, this discrepancy can be understood only by these computational analyses that we did using finite element model, so the understanding obtained from then this approach of combining experimental results and the computational analysis is very much significant in selecting suitable material for the thermal protection system of the supersonic vehicles experiencing the erosion wear.

So, this particular study proposes or demonstrates necessary guidelines for assessing thermal erosive structural stability of materials utilising a novel approach of coupling experimental results and computational analysis, so I hope you like this part of this lecture, thank you.