Analysis and Optimization of Zirconium-2 Alloy'by Using Finite Element Analysis

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Abstract: The paper is presents the understanding the factors that contribute to U^Pb discordance in zircon is essential for interpreting isotopic data and for assessing the validity of concordia intercept ages. Modification caused by interaction with metamorphic fluids is often cited as a primary means by which significant or even complete isotopic resetting of U^Pb systematics in zircon might be achieved under sub solidus conditions. Conventional ion microprobe analysis of sectioned and polished grain surfaces indicates that fluid interaction resulted in minor disturbance of U and Pb in zircons (both normal and reverse discordance) with limited displacement along a chord with a lower intercept that coincides with the timing of fluid infiltration. Although zircon underwent some radiogenic Pb redistribution during fluid interaction, infiltrating fluids resulted in minimal grain-scale isotopic modification of zircon. Based on ion probe depth profiling results, we propose that limited normal discordance observed in the conventional ion microprobe zircon analyses, in this case, is controlled by an analytical mixture of reset and/or recrystallized zircon along penetrative micro-fracture networks with that of adjacent unaffected zircon.

I. INTRODUCTION

Failure of components occurs at low stress values than the ultimate or yield strength of the material due to the application of time varying cyclic loadings. This phenomenon is called fatigue. Basically crack initiation and crack propagation are the main cause of fatigue failure of components. First of all due to cyclic loading components become unstable and crack initiation takes place and after that crack propagation results in sudden failure. Calculation of total fatigue life is done by adding the life of crack initiation and the life of crack propagation. It is not possible to calculate the fatigue life by separating the two phases of crack i.e. by separating initiation of crack and propagation of crack by any method.

Generally, failure of Zircaloy-2 through fatigue or other fracture modes is caused by cracks initiated from prominent defects. If these defects are eliminated, performance is improved.

Major defects in Zircaloy-2 that influence fatigue resistance are porosity and inclusions, especially oxide films. Porosity has been shown to be the most detrimental defect. For a given application, in addition to the fatigue life of castings with various defect levels, it is important to consider the maximum porosity, as well as the largest pore size that can be tolerated.

It can be seen that, in addition to their large number, Fatigue behaviour is controlled by these factors in a hierarchical manner.

A. ***Effect of Ductility/Plasticity:*** When the ductility of the material plays an important role, EPFM (Elastic Plastic Fracture Mechanics) is a very much precise substitute to LEFM (Linear Elastic Fracture Mechanics) in evaluation of the active properties of Zircaloy-2. LEFM correlates crack growth rates resulting from an applied cyclic load (da/dN) to the stress intensity factor ΔK; this is given by:

$$\frac{da}{dN} = C\,(\Delta K)^m\,,$$

Where da/dN is the crack growth increment per loading cycle, ΔK is the factor of stress intensity (Kmax-Kmin), and C and m are functions of the stress ratio, frequency, environment, temperature, material variables etc.

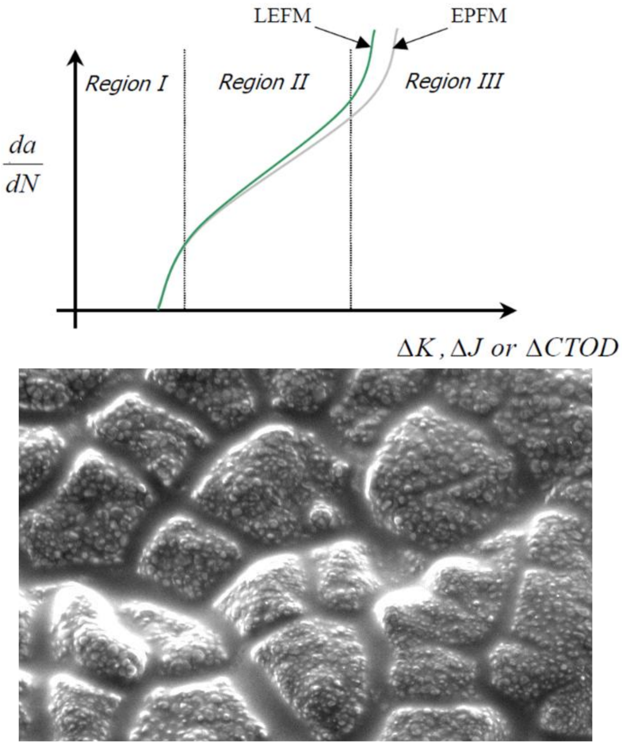

Figure 1 :LEFM vs. EPFM in high plasticity conditions.

In graphical form this relationship is seen in Figure.1.1. Regions I, II, and III correspond to the initiation, propagation, and final failure in crack evolution. It is important to point out that for longer crack length; the plasticity region present in front of the crack becomes more and more significant. Therefore, because of yielding, LEFM becomes less and less accurate at higher ΔK values, and elements of EPFM, such as the J-integral or CTOD (Crack Tip Opening Displacement) need to be considered to obtain realistic representations of the upper Region II, Region III and fracture toughness of the material. K_{IC} values from LEFM evaluations underestimate the behaviour of the material. A more accurate approach to both FCGR curves and fracture toughness should consider a cyclic J–analysis using the load-displacement data from the FCGR experiments.

B. ***Effect of Residual Stress:*** Zircaloy-2 is heat treated by quenching solution treatment which is monitored at a temperature approximately 1000°F. As a result the introduction level of residual stress in the components (or samples) is significant. On the surface of sample, nature of the residual stresses is compressive, which cools first, while in the centre of sample, nature of the residual stress is tensile, which cools later. Quenching treatment is processed on the whole sample to balance the tensile stress and compressive stress, which results zero net effective stress on the sample. Subsequently for enhancement of the strength of the sample without having any effect on the residual stresses in the part aging treatment is processed on the sample.There are several ways to eliminate residual stresses, such as thermal (annealing), mechanical (mechanical deformation), and thermo-mechanical (so-called “up-hill” quench). For Zircaloy-2 the last procedure is the most successful one, in terms of both eliminating the residual stresses and also preserving the shape and the mechanical properties of the part. Since the elimination of residual stresses is not always practical, ways to lucidly deal with it are required. There is a very significant contribution of residual stresses on fatigue crack growth behaviour of several alloys. This is true for Zircaloy-2, aluminium, super alloys, titanium, steels, and not only in castings, but also in forgings, extrusions, etc. This situation represents tests conducted on compact tension specimens. It can be noticed that the thresholds are shifted towards higher values of ΔK, due to the significant closure effects that result due to occurrence of residual stresses, in addition to the effects of the alloy microstructure. For high residual stresses, the thresholds can be increased by as much as a factor of two. It is important to note that residual stresses also affect the fracture toughness K_{IC} to a lower degree, i.e., up to 20-25%. On the other hand, for centre-cracked tension specimens, thresholds are predicted to be lower than those obtained in the absence of residual stresses (in these specimens the notch is located in a region of tension as opposed to a region of compression in compact tension specimens). In conclusion, residual stress is a major issue that cannot be ignored, and mathematical and experimental ways to account for it need to be created. In this sense, ASTM guidance should also be developed and added to the existent standard procedures for measuring crack growth rates. Fatigue crack growth response of Zircaloy-2 is mainly affected by alloy microstructure and residual stress. Fatigue crack growth behaviour is prominently affected by residual stress at low ΔK.

C. ***Fracture Mechanics:*** Fracture mechanics is a branch of science involving with micromechanics and strength of materials. Fracture mechanics is applied in order to obtain the fracture parameters of a cracked components or specimens, creating a singular stress field at the tip of the crack. Fracture toughness describes the ability to resist fracture and depends on component dimension, loading and material properties at the operating conditions. In practice, steel components are in many cases too large and too expensive to be tested as such in their operating conditions for their fracture characteristics. Thus, it is more beneficial to divide the fracture toughness determination in two stages: firstly, the determination of the fracture toughness of the material as a function of the test temperature and other operating conditions, and secondly application of a scaling dependent factor to obtain the fracture toughness of the component or its weakest part. Specimens that can be tested in laboratories and are inexpensive enough to be broken in large numbers are used for the first stage of the fracture toughness determination. Currently, there exist numerous standards for the fracture toughness testing of metallic materials. Common to all standards is a requirement of large enough specimen size in order to obtain test results dependent solely on the material properties, not on the dimension or the size of the specimen. Problems are encountered with the size requirement. Usually low strength materials have high fracture toughness and so the minimum required specimen size for those materials may be very large, in some cases of the order of several meters. This leads to the need of larger testing machines which increases costs. On the other hand, in some cases due to availability of material and manufacturing process the size of standard specimen is limited. For example, irradiated specimens must be small due to limited volume of the irradiation chambers and strong neutron flux gradients. Thus, the maximum irradiated specimen size becomes far smaller than required by the standards. Due to the above mentioned reasons, testing of standardized specimens is in some cases uneconomical or impossible and smaller specimens have to be tested to get an idea of the fracture toughness level. These results in a problem of obtaining a geometry independent result from test results obtained with very small specimens, i.e. the removal of the geometry effect. There are two, parallel ways to investigate the geometry effect on fracture toughness: experimental and computational analysis, the latter referring often to Finite Element Method (FEM). This project work includes both types of approaches. Experimental fracture toughness values have been determined for specimens with varying thickness (B), varying ratio of crack depth to specimen width (a/W) or varying flaw geometry from through the thickness to elliptical surface cracks. Extensive finite element analyses (FEA) have been applied for models with geometries ranging from standardized specimens to plates with surface flaws, having specimen thickness, crack size and material strain hardening exponent as parameters. Also the effects of side grooving have been studied. For the determination of fracture toughness of metallic materials using the following parameters such as K, J, and CTOD (δ).

II. ZIRCALOY-2

Zircaloy-2 is a zirconium-tin alloy developed for use in water cooled nuclear reactors. It possesses good corrosion resistance to high-temperature water, excellent nuclear characteristics, and sufficiently good mechanical properties for use as a structural material in reactor cores and as a fuel element material. The mechanical and physical properties of major concern for reactor components are as follows: 1. Short-time strength and ductility. 2. Long-time strength and ductility. 3. Low-cycle fatigue. 4. Physical properties such as elastic modulus, coefficient of thermal expansion, Poisson’s ratio, and thermal conductivity.

Zirconium and its alloys (e.g. Zr-Sn alloys Zircaloy-2 and Zircaloy-4) are widely used in the nuclear industry because of their low neutron capture cross-section, good corrosion resistance in hot water, and reasonable mechanical properties. The nominal composition of Zircaloy-2 is Zr, 1.2-1.7wt% Sn, 0.07-0.2wt% Fe, 0.05-0.15wt% Cr, 0.03-0.08wt% Ni, 1400wt ppm oxygen. The sum of Fe, Ni and Cr must be within 0.18-0.38%. The addition of Cr, Fe and Ni additives can improve the corrosion resistance of Zr, while maintain the good mechanical properties.

Composition of Zircaloy-2: A multi-faceted alloy of sponge Zirconium is basically known as Zircaloy-2 which contains the following major components and impurities which is employed for reactor-grade material:

Element \Weight (%):

Major Components - Tin\1.3-1.8, Ferrous\0.08-0.21, Chromium\0.05-0.15, Nickel\004-0.09.

Impurity – Aluminium\0.0076, Boron\0.00006, Carbon\0.0275, Cadmium\0.00007, Cobalt\0.0025, Copper\0.0052, Hydrogen\0.0025.

Zircaloy-2 will allow an improved understanding of the plastic deformation of Zr alloys in general, and the prediction of in-reactor deformation of tubes made by different manufacturing routes. For instance, the calendric tube for Advanced CANDU Reactor has different dimensional requirements than the existing one, and this demands a change in the manufacturing route

III. MECHANICAL PROPERTIES

Quenching from above the hydrogen solubility temperature lowers the transition temperature and increases the transition range. Experimental data indicating decreased impact resistance with increased hydride precipitate are presented in

Figure 3: Tensile properties are not so dependent on hydrogen content.

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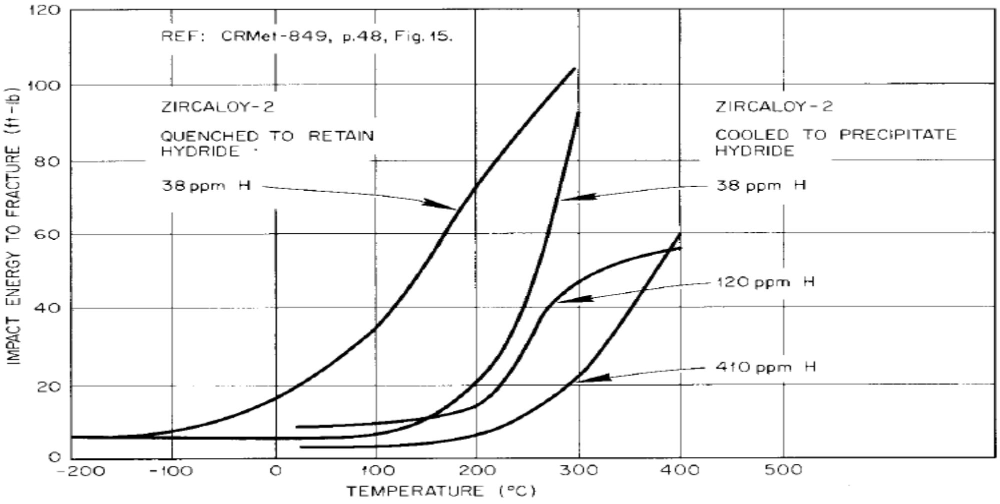

Figure 3: Tensile properties are not so dependent on hydrogen content.

Mechanical properties of the Zircaloy-2 for different processing conditions.

Material	Hardness	Tensile strength (MPa)	Yield strength (MPa)	% elongation at break
Zircaloy-2	182	499	331	25
75% RTR	247	591	541	6.4
85% RTR	269	679	666	5.5
75% CR	257	800	765	5.07
85% CR	282	891	835	4.1

IV. TENSILE PROPERTY

Zircaloy-2 shows the typical stress-strain relationship of nonferrous metals (Figure.3.2.). Since tensile properties are dependent on specimen history, a so-called "base-annealed" condition (annealed at 1382°F in vacuum for approximately 20 hr. and furnace cooled in vacuum) is used here as a reference condition.

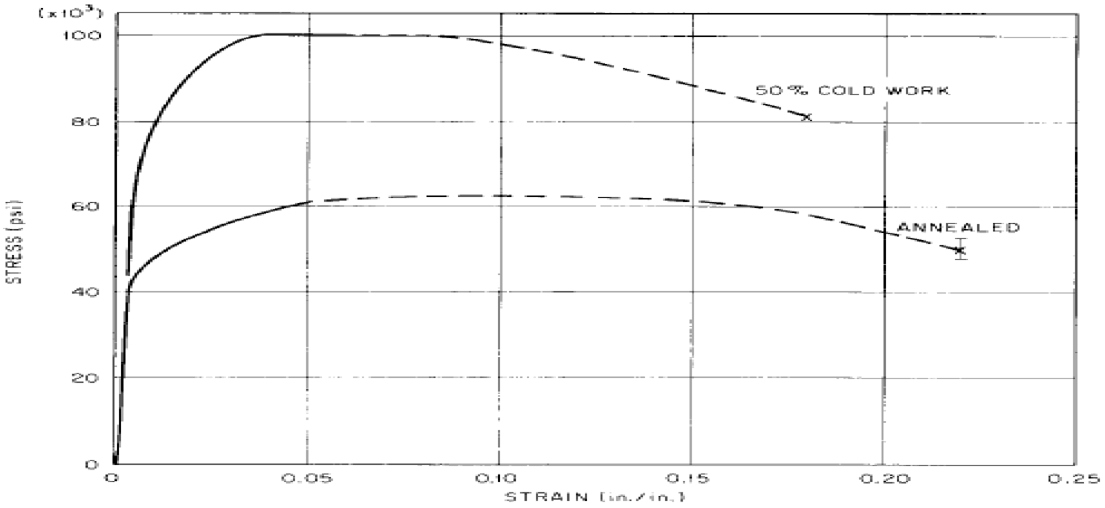

Figure 4: Typical Stress-Strain Relationship For Zircaloy-2

V. FATIGUE PROPERTIES

According to fatigue-test data Zircaloy-2 is very much sensitive with notch. Effect of notch. Fatigue strength for lifetimes less than 10^6cycles does not affected by adjustment of notch geometry ranging in K_t= 3 to 9; where, K_t is the theoretical stress concentration factor. Stress concentration magnitude, temperature and orientation do not affect the strain-fatigue properties of Zircaloy-2 significantly.

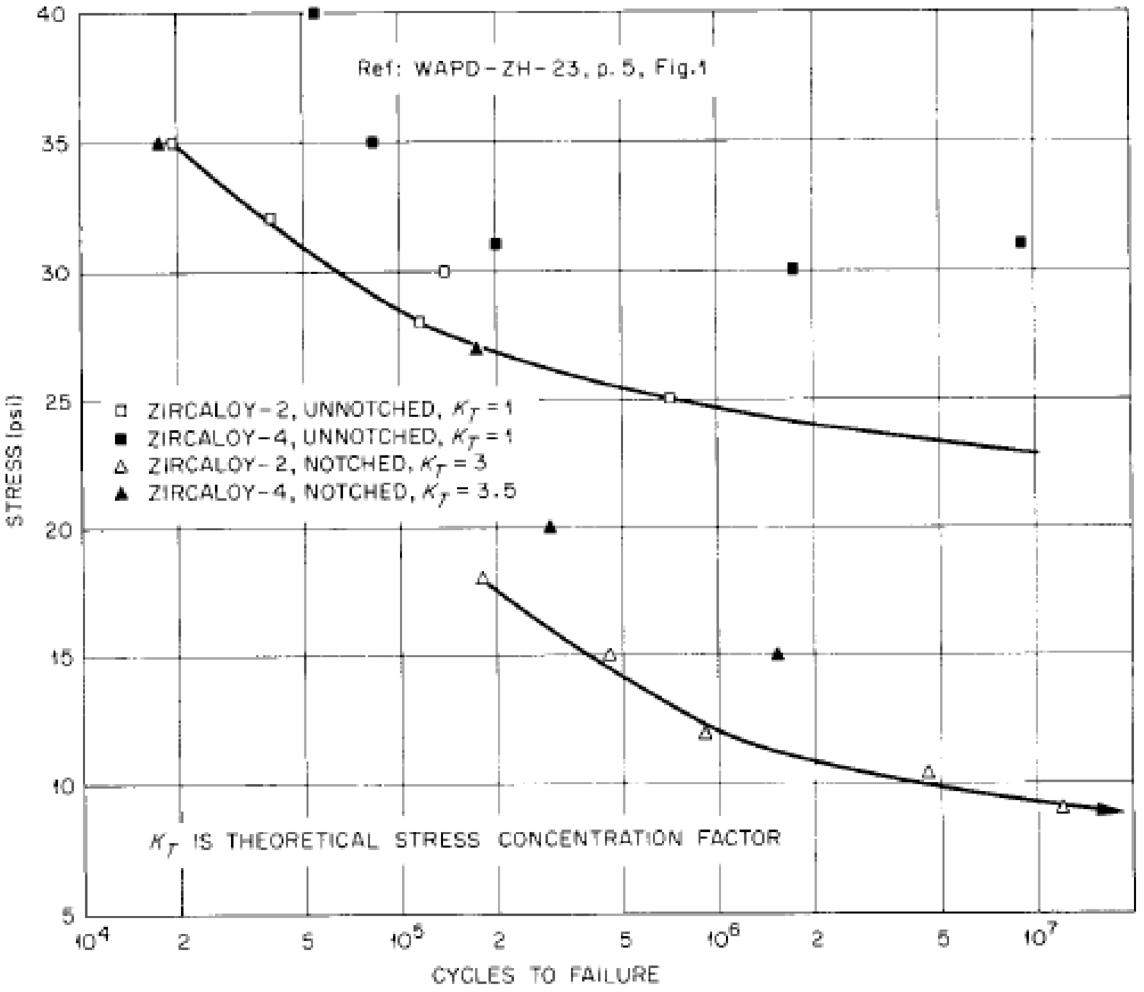

Figure 5: Reverse-Bend Stress-Fatigue Data for Base-Annealed Zircaloy-2 and Zircaloy-4 Tested at 600

VI. CREEP PROPERTIES

Two major variables are there first impurity content and second temperature. Other data indicates that in 14 to 25% cold worked Zircaloy-2, third stage creep occurs at almost 2% of total plastic strain at 16500 psi and 300℃ and at almost 0.08% of total plastic strain the first stage creep seems to be occur. Thus, the third stage creep will be happen after a long time period approximately 48 years for a 5×10^{-6}%/hr. secondary creep

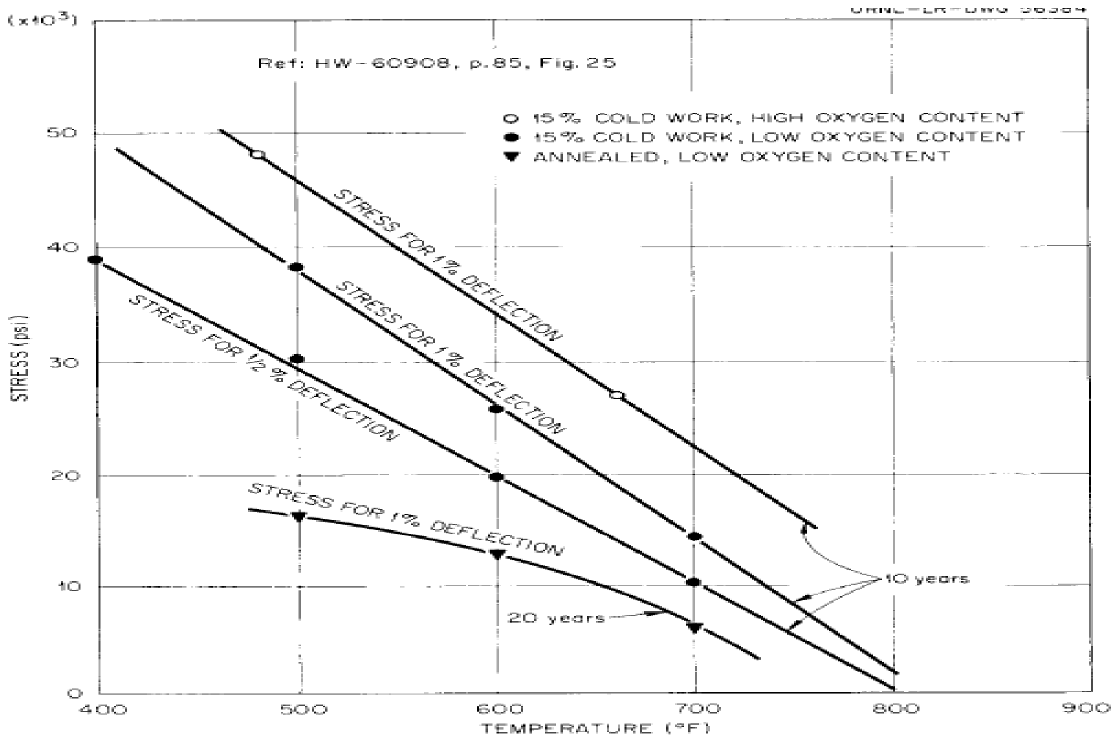

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Figure 6: Long-Term Creep Predictions for Zircaloy-2

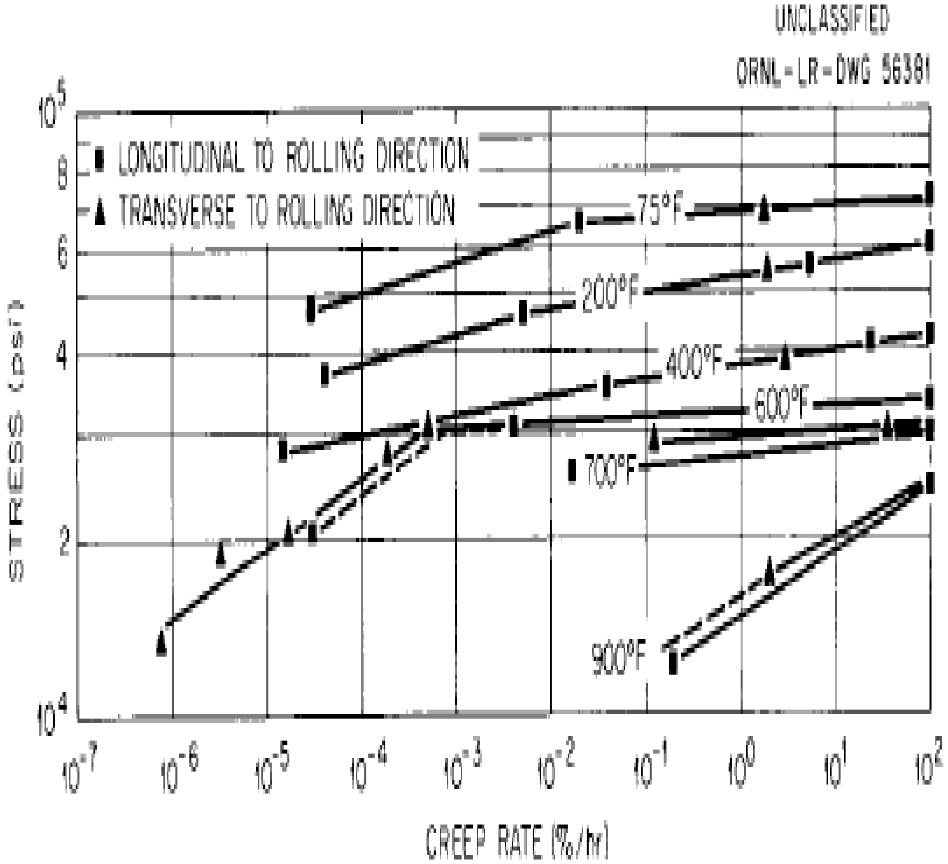
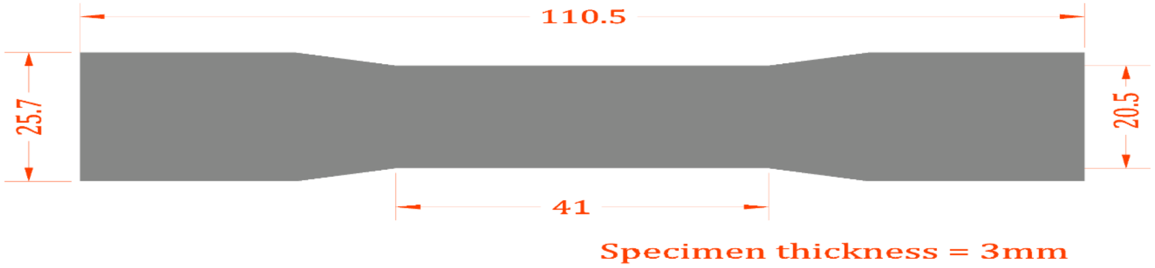


Fig-7 Long-Term Creep Predictions for Zircaloy-2

VII. ANALYSIS METHODOLOGY

The products which is subjected to repeated cyclic loading specified of failure termed as fatigue failure.Varying or repeated loads on repetitive stress for a long time duration changes the microscopic structure of component which resulted into crack formation that origins the breakdown.. Basically we use to do fatigue simulation for following factors:***a.***Desired product life,***b.***Optimization of shape and size,

c. Optimization of material consumption.Ansys is a tool containing non-destructive simulation process to simulate fatigue life which is governed by equation of fatigue.



Fatigue is analysed by two methods in Ansys:**A.**Strain life.**B.** Stress life.

Strain life is basically characterized for low cycle fatigue and it can be directly measured. Fewer than 10^5 (100000) cycles is termed as low cycle fatigue. Required input for strain life is the total strain (Elastic-plastic).

Strain life relation equation is shown below:

$$\frac{\Delta\varepsilon}{2} = \frac{\sigma_f}{E}\left(2N_f\right)^b + \varepsilon_f\left(2N_f\right)^c$$

$\Delta\varepsilon/2$ → total strain amplitude, σ_f→ fatigue strength coefficient, N_f → numbers of cycles to failure, ε_f→ fatigue ductility coefficient → modulus of elasticity, b → fatigue strength exponent (Basque's exponent), c → fatigue ductility exponent

To relate the strain to stress we use Neuber's rule, which is shown below:

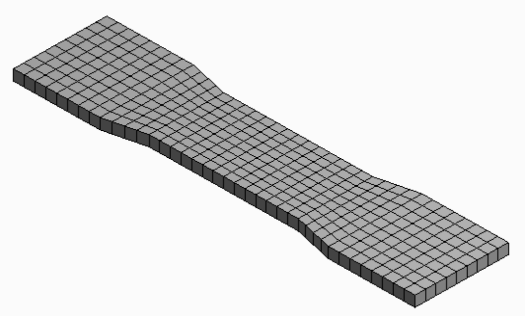
$$\varepsilon\sigma = K_t^2 eS$$

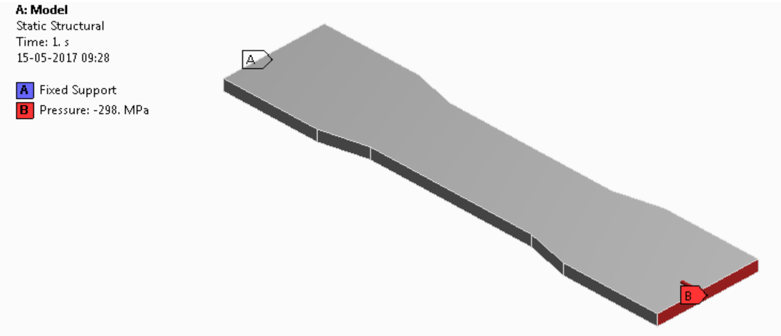
ε → total strain, σ→ local stress, K_t → elastic stress concentration factor, e→ nominal elastic strain, S→ nominal elastic stress

Stress life is basically based on stress-cycle curves (S-N curves). Stress life is not distinguished between initiation and propagation. Stress life is fully concerned with total fatigue life. Traditionally stress life deals with high cycle fatigue and high numbers of cycles that is greater than 10^5 (100000) cycles.

A. Geometry, Mesh and Boundary Conditions

A standard specimen of gauge length of 40mm and gauge width of 20 mm is modeled with the help of design modeler of ANSYS. While overall job length is 110 mm and job width is 25 mm and job thickness is 2.5 mm. Then auto meshing is done by mesh tool. Boundary conditions and loadings are applied. One end of specimen having fixed support while, other end having loadings as pressure. We have done fatigue analysis for un-notched and notched specimen both for all different processing conditions of Zircaloy-2.





B. *Mean stress correction for stress life*

- Soderburg mean stress correction theory:

$$\frac{\sigma_{alternating}}{S_{endurance\ limit}} + \frac{\sigma_{mean}}{S_{yield\ strength}} = 1$$

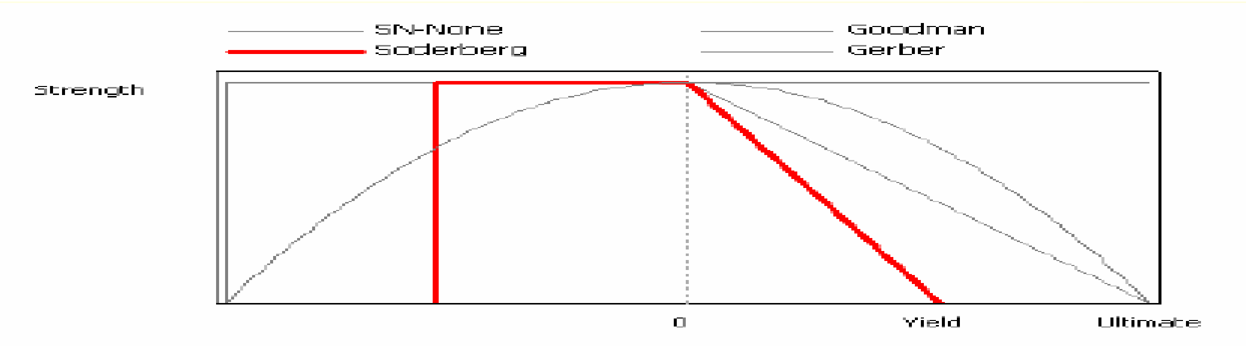


Figure 9: Soderburg Mean Stress Theory.

- Goodman mean stress correction theory:

$$\frac{\sigma_{alternating}}{S_{endurance\ limit}} + \frac{\sigma_{mean}}{S_{ultimate\ strength}} = 1$$

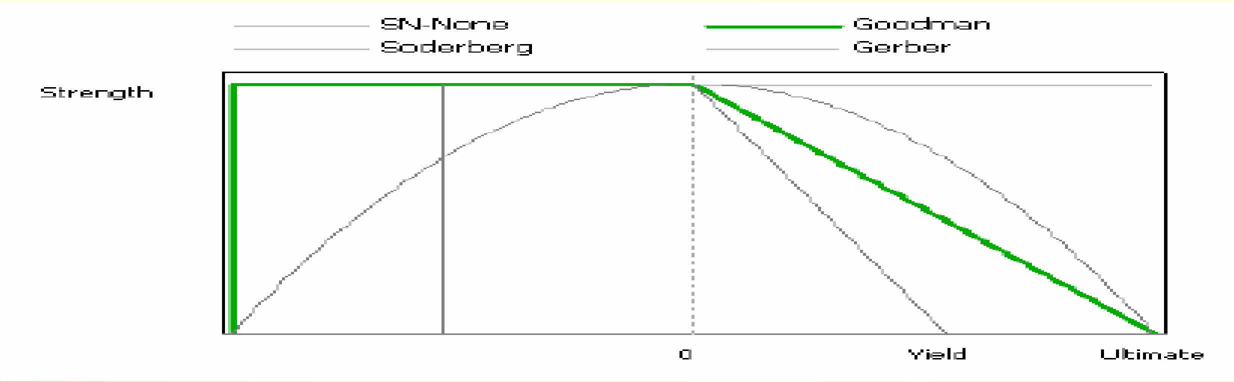


Figure 10: Goodman Mean Stress Theory.

- Gerber mean stress correction theory:

$$\frac{\sigma_{alternating}}{S_{endurance\ limit}} + \left[\frac{\sigma_{mean}}{S_{ultimate\ strength}}\right]^2 = 1$$

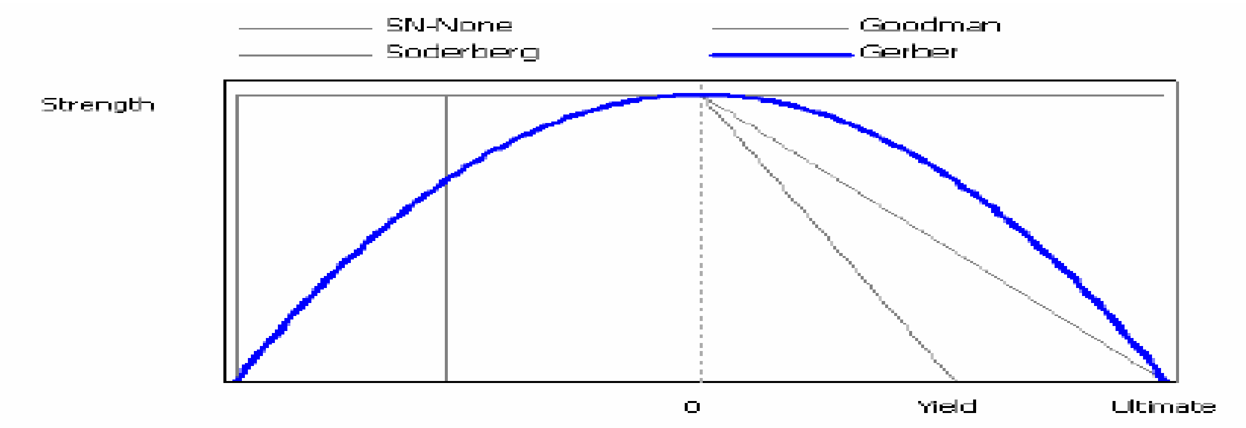


Figure 11: Gerber Mean stress Theory.

C. *Mean stress correction for strain life*

- Morrow's method:

$$\frac{\Delta\varepsilon}{2} = \frac{\sigma_f + \sigma_{mean}}{E}\left(2N_f\right)^b + \varepsilon_f\left(2N_f\right)^c$$

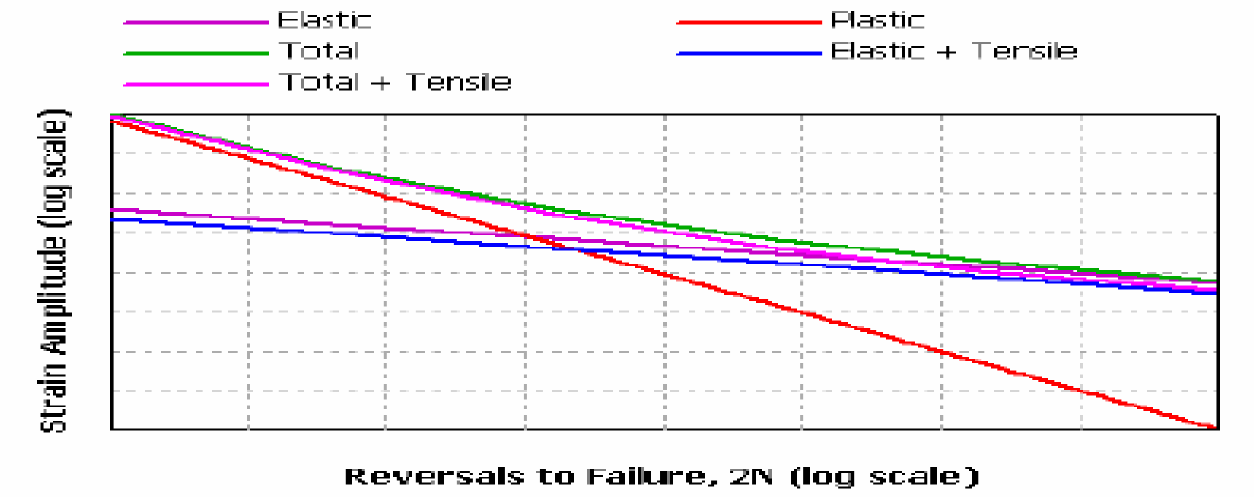


Figure 12: Morrow's Method.

- Smith, Watson and Topper (SWT) method:

$$\sigma_{max}\frac{\Delta\varepsilon}{2} = \frac{\sigma_f^2}{E}\left(2N_f\right)^{2b} + \sigma_f\varepsilon_f\left(2N_f\right)^{b+c}$$

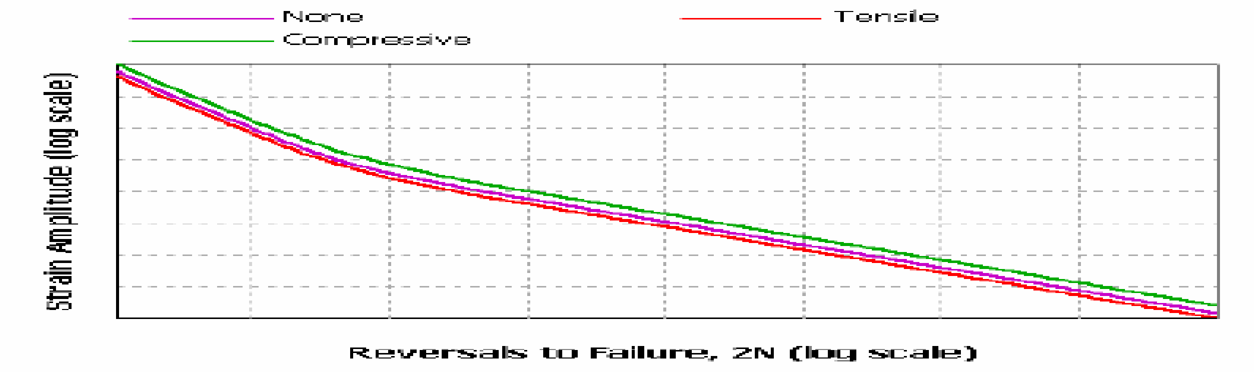


Figure 13: Smith, Watson and Topper (SWT) method.

I. FEA RESULTS

Mechanical property of 75% RTR Zircaloy:

Young’s modulus = 96 Gpa, Poisson’s ratio = 0.3, Tensile yield strength = 541 Mpa, Compressive yield strength = 541 Mpa, Ultimate tensile strength = 591 MPa

Results:

Equivalent stress:

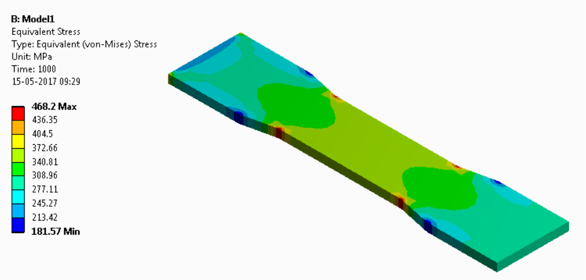


Figure 14: Equivalent stress of 75% RTR Zircaloy.

Equivalent strain:

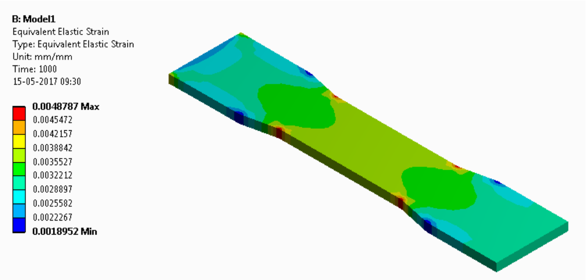


Figure 15: Equivalent strain of 75% RTR Zircaloy.

Fatigue life:

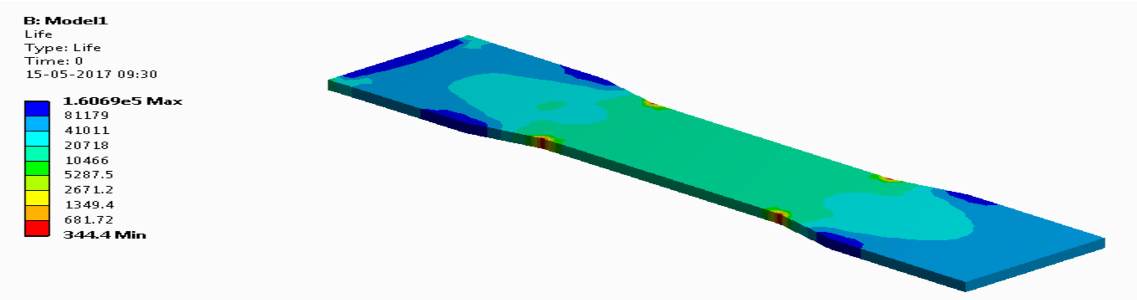
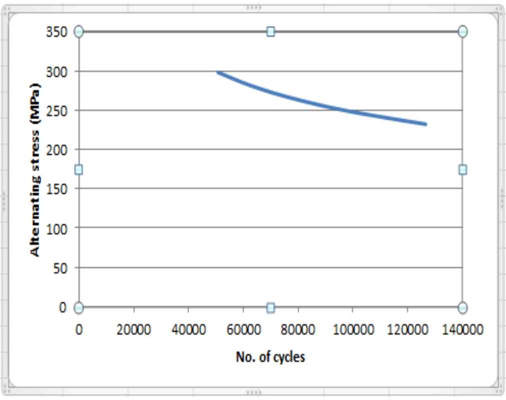
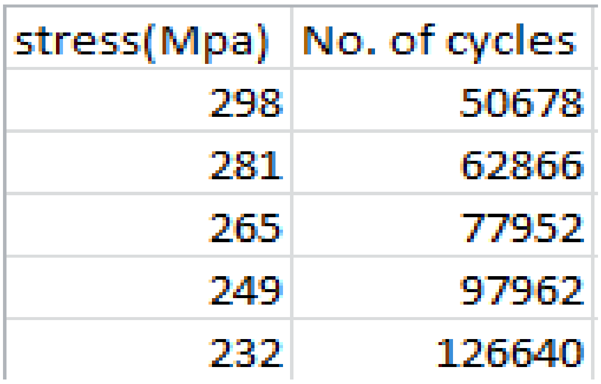


Figure 16: Fatigue life of 75% RTR Zircaloy.

S-N curve:



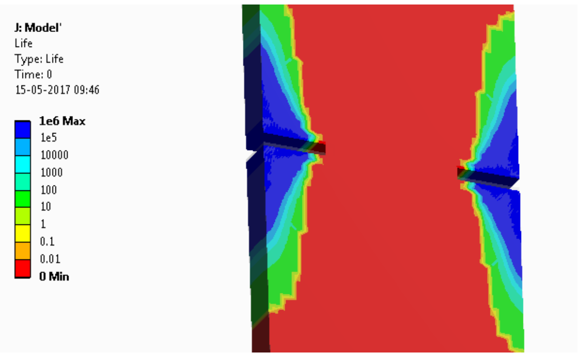


stress(Mpa)	No. of cycles
298	50678
281	62866
265	77952
249	97962
232	126640

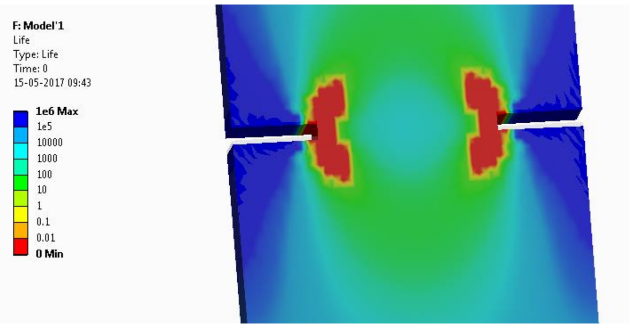
Fatigue analysis for notched specimen:

Fatigue life for Zircaloy-2:

Fatigue life of Zircaloy-2 for notched



Fatigue life of 75% RTR Zircaloy for notched



Comparative S-N curve for notched specimen of different processing materials of Zircaloy2:

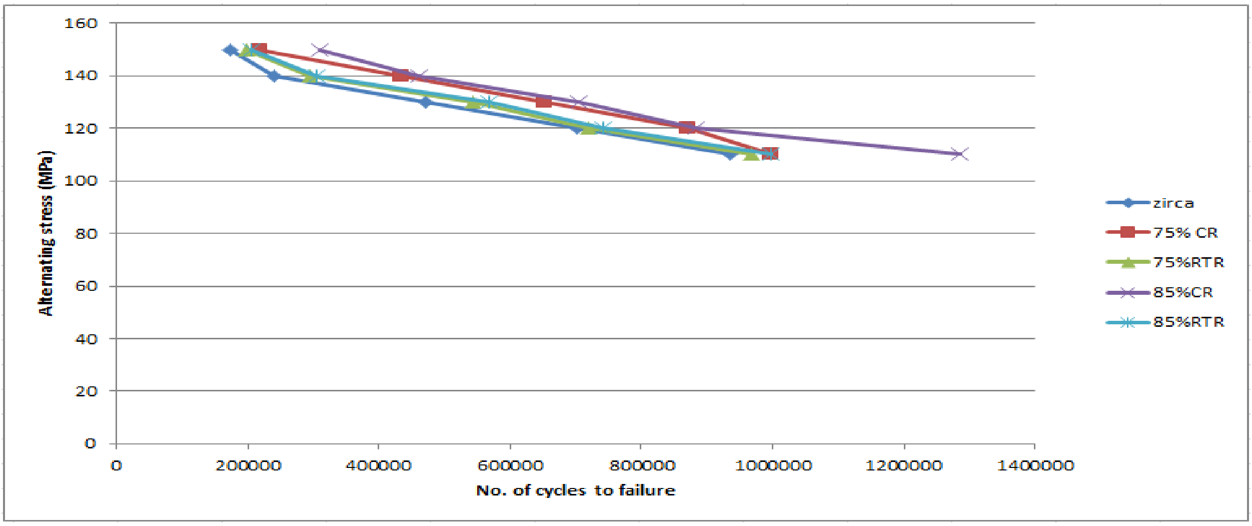


Figure 17: Comparative S-N curve for different processing materials of Zircaloy-2 for notched specimen.

II. CONCLUSION

In this dissertation report, standard specimen of Zircaloy-2 material was studied in order to clarify the effect of fatigue on notched surface and without notched surface. Following conclusions are made in this project by using ANSYS software:The fatigue analysis of standard specimen of Zircaloy2 has been conducted.S-N curve has been obtained for alternating stress.Fatigue test data show that Zircaloy2 is notch sensitive.Analysis of 3-D cracks has been performed and S-N curve obtained for cyclic loading.For Zircaloy-2 with kinematic behaviour, it is considered that cyclic hardening properties should be used for all simulations of crack closure under variable amplitude, especially for long crack lengths. Monotonic loading properties might be employed under constant amplitude loading and elasto-plastic conditions should be avoided.

Study of fracture behaviour of materials is important as the materials may be subjected to extreme conditions like high temperature, high loading condition etc. In design of large structure, the measurement of fracture toughness is very typical due to their large sizes, therefore, the use of different scale specimens like compact tension and three point bending can be used to measure the effect of change in specimen dimensions.

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