B. TECH. PROJECT REPORT

On

Finite Element Simulations of Tensile Deformation Response of notched-Metallic Glass Samples

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DISCIPLINE OF MECHANICAL ENGINEERING
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Finite Element Simulations of Tensile Deformation Response of notched-Metallic Glass Samples

A PROJECT REPORT

Submitted in partial fulfillment of the
Requirements for the award of the degrees
of
BACHELOR OF TECHNOLOGY
in
MECHANICAL ENGINEERING

Submitted by:
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Guided by:
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INDIAN INSTITUTE OF TECHNOLOGY INDORE
December -2018

CANDIDATE'S DECLARATION

We hereby declare that the project entitled **Finite Element Simulations of Tensile Deformation Response of notched-Metallic Glass Samples** submitted in partial fulfillment for the award of the degree of Bachelor of Technology in Mechanical Engineering completed under the supervision of **Dr. Indrasen Singh,** at IIT Indore is an authentic work. Further, we declare that we have not submitted this work for the award of any other degree elsewhere.

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Signature and name of the student(s) with date

CERTIFICATE by BTP Guide(s)

It is certified that the above statement made by the students is correct to the best of my knowledge.

Signature of BTP Guide(s) with dates and their designation

Preface

This report on "Finite Element Simulations of Tensile Deformation Response of notched-Metallic Glass Samples" is prepared under the guidance of Dr. Indrasen Singh.

Recent experiments and molecular as well as continuum simulations have shown that presence of notch in metallic glass (MG) samples enhance the tensile ductility. These studies were focused on analyzing the tensile response of single edge and double edge notched-MG samples. However, the presence of multiple notches on the surfaces of MG samples have not investigated. In particular, spacing of the notches with respect to intrinsic material length associated with flow defects such as shear transformation zones (STZs) may have marked effect of mechanical response of MG samples. Therefore, continuum analysis of tensile response of MG samples with multiple notches is performed using thermodynamic consistent non-local plasticity model for MGs in this study. The effects of notch spacing, ligament length and intrinsic material length are investigated.

The authors have tried to the best of their abilities and knowledge to explain the content in a lucid manner. To this end contour plots and figures are also included to make report more illustrative.

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Abstract

Since their invention, metallic glasses (MGs) have been a great interest of research for many scientists because of their unique and superior mechanical properties. The first metallic glass ($Au_{80}Si_{20}$) was manufactured by Duwez at the California Institute of Technology in the year 1960 through rapid quenching by employing cooling rate around 10^6 K/s. This much high cooling rate was needed so that crystallization could be suppressed and metal in amorphous state could be produced. This restricts the size of MGs, hence they were produced in the form of thin films. It was found after considerable research that the required cooling rate is much lower in multy-component systems opening ways to synthesize MG as thick as 10. These MGs are referred to as bulk MGs. Owing to the glassy nature these materials hold attractive combination of chemical, electrical and mechanical properties such as ,excellent corrosion resistance, very high yield strength and strain and good electrical conductivity. This has made them a potential candidate for various engineering applications including in nanotechnology, sporting equipment's, electronic components and for medical purposes.

Nevertheless, MGs do not show any ductility under tensile loading and fail catastrophically due to uncontrolled propagation of crack inside a shear band. Thus, lack of tensile ductility is the 'Achilles heel' in their inception in actual engineering applications. Recent experiments have shown that MGs can exhibit a significantly large tensile ductility for initial size below 100 nanometer. Also, it has been observed that the presence of notches plays a significant role in increasing the ductility of Nano-sized samples.

It has been observed that the plastic zone size attains a saturation level when a dominant shear band is formed. This size scale depends on the intrinsic material length which captures the effect of material composition in finite element simulations.

In this work, finite element analysis of tensile loading on Nano-sized notched MG specimens are performed using a thermodynamically consistent non-local plasticity model to understand the effect of the intrinsic material length and, position and radius of notches.

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Chapter1. INTRODUCTION

1.1 Amorphous and crystalline solids -:

Amorphous solids -: The solids in which the constituent particles of matter are arranged in a random manner are called amorphous solids. It is a non-crystalline solid with no proper arrangement of atoms in the solid lattice. In other words, we can define amorphous solids as materials which don't have a certain organized arrangement of atoms and molecules. Most solids are amorphous in nature and are utilized in many sectors as well. One of the most common examples of amorphous solids is glass, which is used widely in the manufacturing sector.

Crystalline solids -: The solids in which the constituent particles of matter are arranged and organized in a specific manner are called Crystalline Solids. These solids contain crystals in their structure and each crystal has definite geometry. Adding further, as crystalline solids have low potential energy, they are the most stable form of solids. Almost all solids fall in the category of crystalline solids including metallic elements (iron, silver, and copper) and non-metallic elements (Phosphorus, Sulphur, and iodine). Also several compounds like sodium chloride, zinc sulfide and naphthalene build crystalline solids.

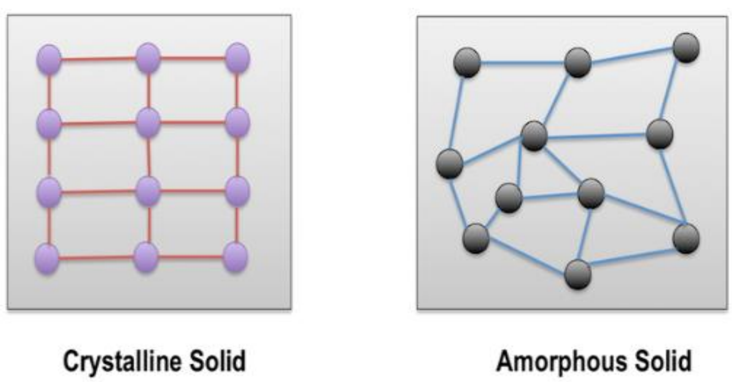


Figure 1-: Arrangement of Atoms

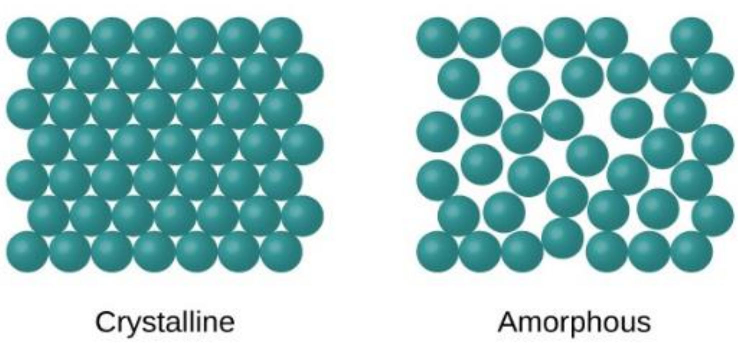


Figure 2-: Shape of Crystalline and Amorphous Solids

1.2 What are Metallic Glasses?

Metallic glasses are amorphous metal. When the molten metal alloy is cooled rapidly, they solidify in disorderly fashion thus imparting the amorphous structure. MGs offer combination of various mechanical properties which makes them a suitable candidate for building materials.

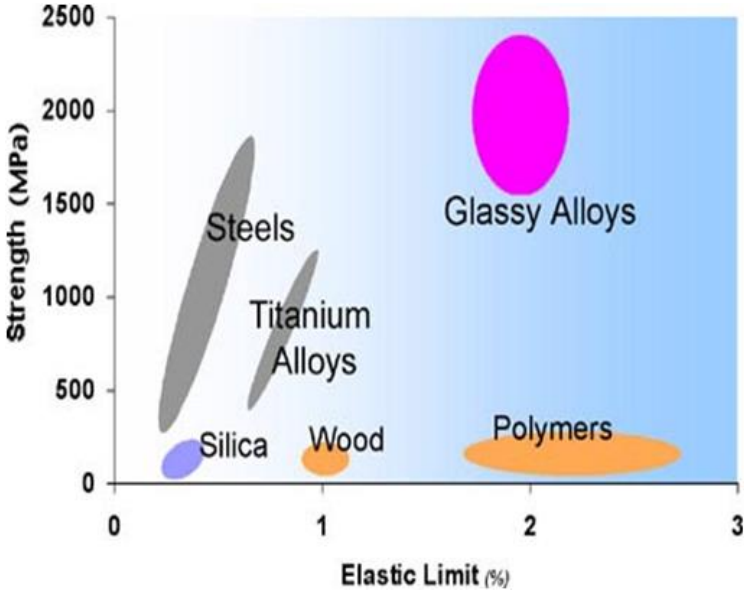


Figure 3-: Strength and Elastic strain plot for different materials.

With no crystal defects, metallic glasses have a lot of remarkable properties, which promise a lot of applications in engineering. However, the biggest hurdle to achieve this goal is the lack of ductility due to an uncontrolled propagation of dominant shear bands. Various strategies have been developed for increasing the ductility such as designing MG composites, using nano-scale samples and introducing notches.

A good tensile ductility can be achieved when the sample size is taken in the order of 100 nm. For example, tensile experiments performed on 100 nm Zr-based MG specimen showed plastic strain up to 4.5 % and final failure by either necking or stable growth of the shear band. In samples which failed vie necking, it was found that these samples had surface unevenness in the form of shallow notches and concluded that these notches served as stress concentrators and were responsible for triggering necking.

1.3 Applications

1.3.1 Electrical and Electronics -: Since metallic glasses have high electrical resistance, they are used to make accurate standard resistance, computer memories and magnetic resistance sensors.

Figure 4.1 :- Pressure sensor

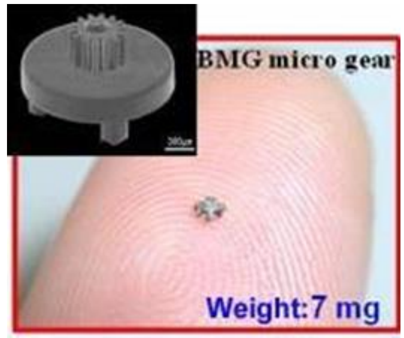


Figure 4.2 :- Micro gear

<u>1.3.2 Nuclear reactor engineering</u> -:(a) The magnetic properties of metallic glasses are not affected by irradiation and so they are useful in preparing containers for nuclear waste disposal and magnets for fusion reactors.
(b) Chromium and phosphorus-based metallic glasses have high corrosion resistance and so they are used in the inner surface of the reactor vessels.

<u>1.3.3 Biomedical Industries</u> -:(a) Due to high resistance to corrosion, metallic glasses are suitable for cutting and making surgical instruments.
(b) They may also be used as prosthetic materials for implantation in the human body.

Figure 4.3:- Titanium-based BMG alloy tooth implant

<u>1.3.4 Space Technology</u> -:
NASA is developing bulk metallic glass gears and power Transmission systems as they have seen in researches that Metallic glass doesn't wear out much even at a much lower temperature of -173 degree centigrade these characteristics make them a better replacement for steels.

Figure 4.4-: (More than 3 million cycles were achieved at less than –100 °C with dry lubricated hybrid gearbox).

1.3.5 Other Applications -: (a). They possess high physical and tensile strength. They are more superior than common steels and thus they are useful as reinforcing elements in concrete, plastic, and rubber.

(b). Strong Ribbons of metallic glasses can be used for simple filament winding to reinforce pressure vessels and also to construct large flywheels for energy storage.

(c). Due to their good strength, high ductility and good corrosion resistance, they are used to make razor blades and different kinds of springs.

(d). Since metallic glasses have soft magnetic properties, they are used in tape recorder heads, cores of high-power transformers and metallic shields.

(e). Superconducting metallic glasses are be used to produce high magnetic fields and magnetic levitation effect.

Figure 4.5: -Tungsten + Vitreloy composite KEP rods

Figure 4.6: -Golf club, face material Zr-based MG

1.4 Failure theory of metallic glass

1.4.1 Shear bands

Shear banding is proof of plastic instability that localizes shear strains in a thin band when the material is plastically deformed. There are two theories that explain the formation of shear bands in amorphous metals.

1.4.2 Shear Transformation Zones Theory

For crystalline materials, the elementary process that generates shear strain is gliding of dislocations. But metallic glasses do not have such well-defined defects but still are capable of plastic flow. To explain this, Argon proposed the concept of shear transformation where a group of atoms undergoes cooperative rearrangement by overcoming the saddle point of an energy barrier. Shear transformation involves a group of atoms undergoing large displacements and the local region of these atoms is often termed as Shear Transformation Zones (STZs). STZ theory states that local motion of STZs around free volume sites pushes surrounding atoms apart along activation paths resulting in dilation and strain softening.

1.4.3 Free-Volume Theory

Total volume in an amorphous metal can be divided into space occupied by dense atomic clusters and the empty space among these atomic clusters. These empty spaces are called free volumes. In free volume regions, inelastic relaxation is possible by local atom rearrangements, without any significant impact on surroundings. These sites are preferred regions at which amorphous structure destabilization is initiated, caused by either temperature or applied stress. Deformation-induced strain softening by mechanical dilation is an important feature of plastic deformation of amorphous metals. When shear is applied, large shear-induced excess free volumes are generated which leads to lowering of deformation resistance, strain softening and thereby strong shear localization.

1.5 Literature Review

Guo et. al.(2007) found that transition in tensile deformation from brittle to ductile can be achieved by reducing sample scale to the order of 100 nm. Guo et. al. recorded huge tensile ductility in range of 23-47% where sample failed via necking or stable growth of a shear based in Zr based MG. Further in samples which failed via necking, Guo et. al. noticed surface unevenness which acted as stress concentrators and triggered necking.
Sha et. al. performed molecular dynamics simulation on Cu-Zr MG samples having pre-existing notches and observed that failure occurred due to dominant shear band formation originating at notch tip irrespective of shape size and orientation of notch. Li and Li(2007) performed atomic simulations of tensile loading on externally notched cylindrical and double-notched rectangular Ni–Zr MG specimens and noted that deformation behavior transition from to ductile occurs when specimen diameter or distance between the notches falls below a critical value and in these situations plastic zones develop due to high-stress concentration in front of notches without forming a dominant shear band.
I. Singh(2016) et. al. conducted continuum mechanics simulations on Cu-Zr based MG sample having a single notch with varying notch depth, radius, and intrinsic length and observed that a dominant shear band is formed when notch is far from the opposite side of specimen. But they

made an important observation that brittle to ductile transition happens when the notch is placed close to the opposite boundary of specimen and the intrinsic length is increased. These results were in agreement with results of molecular dynamics and atomic simulations, also they observed the effect of intrinsic material length which captures effect of composition, that upon increasing the intrinsic length the size of shear band increases which allows for plastic zone to develop freely rather than formation of dominant shear band.

Tanmay(2018) et. al. performed molecular dynamics simulations and I. Singh(2018) et. al. performed continuum mechanics simulations on Cu-Zr based MG specimen having two notches. They made an observation that notches with radius to ligament length ratio greater than 2.5 fail via shear band formation as the notch radius is so large that it starts acting like a plane surface. But they made an observation that when radius to ligament ratio is reduced to 1, plastic strain develops due to interaction of STZs without formation of dominant shear band and necking happens. However they observed that when this ratio is further reduced to 0.33, a V-shaped region was formed where plastic strain develops which later failed via dominant shear band formation.

From the above results it was concluded that the failure mechanism of MG samples depend on the various factors such as size scale of specimen, radius to ligament length ratio of notch and the intrinsic parameter length.

1.4 Scope of Dissertation

1. Effect of presence of multiple notches has not been studied yet.
2. Effect of change in ligament length also has not been studied yet.

Chapter2. Constitutive Model and Modelling Aspects

The objective of current study is to observe the tensile response of a nano-sized Cu-Zr MG sample on introducing multiple notches and on varying the ligament length. To perform this study we will be performing continuum mechanics simulations using a thermodynamically consistent non-local plasticity model proposed by A. Thamburaja(2011).

2.1 Constitutive Model

To perform the simulations, we will be using the model proposed by A. Thamburaja. This model explains how free volume generation propagates inside the shear band. Before moving on to the model, it is necessary to understand a few terms which are used to determine the equation.

2.1.1 Interaction stress, τint: For understanding this let's consider an example of a wire carrying electric current. This wire has a magnetic field around it which can interact with its surroundings and when another wire carrying current is brought near it then their magnetic fields interact with each other. Similarly, STZs have field of their own which interact with each other and their interaction determines the development and propagation of shear strain. The stress generated due to interaction between the STZs is called interaction stress and determines the development of plastic strain in the shear band.

2.1.2 Intrinsic Material Length, Lc: In finite element simulations, we don't have a direct method of controlling the composition of the specimen. Therefore we use another parameter which can capture this effect. The intrinsic material length is responsible for controlling the width of shear band and is short ordered of few nanometers, i.e., it plays a significant role when the specimen is in nanometer scale. Increasing Lc increases the width of shear bands and thus enables easier interaction of STZs and higher plastic strain in the region.

Now that we have discussed few basic definitions, we can proceed with understanding how free volume generation happens in the shear bands.

$$\dot{\xi} = K_1 \nabla^2 \xi + \varsigma \dot{\gamma}^p - K_2 \bar{p} - K_3 (\xi - \xi_T) \qquad \text{....(a)}$$

$$\dot{\gamma}^p = \dot{\gamma}_o \left(\frac{f^p}{c} \right)^{1/a} \quad \text{if } f^p = \bar{\tau} - \tau_{int} - \zeta \left(s_2 \left(\xi - \xi_T \right) + \bar{p} \right) > 0, \ \text{where } \tau_{int} = -s_1 \zeta \nabla^2 \xi,$$

$$= 0 \text{ otherwise,}$$

…**(b)**

I- Free Volume Diffusion
When amorphous metals are not subjected to any stress, even then the free volume diffuses throughout the specimen. This diffusion of free volume is dependent on the temperature of the specimen and thus this behaviour can be understood as happening spontaneously in the material, similar to creep effect in certain materials.

II- Free Volume Generation due to Plastic Shearing
When the specimen reaches its elastic limit, the STZs convert into shear bands. If the growth of shear band is controlled, then plastic strain develops in this region.

$$L_c = \sqrt{s_1/c_o}$$ ….**(c)**

From equations (b) and (c), we can observe interaction stress is dependent on intrinsic material length, Lc. When interaction stress reaches negative value, the rate of development of plastic strain increases thereby increasing the rate of free volume generation. So the intrinsic length governs shear bandwidth in MGs.

III- Free Volume Generation due to Hydrostatic Stress
Unlike metals, MG has been found to be affected by hydrostatic stress significantly.

IV- Free Volume Generation due to Structural Relaxation
When amorphous metals are subjected to tensile loading, due to the concentration of stress in a region the free volumes diffuse towards that region collacing together and forming shear bands in those regions.

2.2 Modelling Aspects

A rectangular specimen (100(W)*200(L))nm containing notches at the edge with ligament length or sample thickness Bo and radius R, while S is the spacing between two notches. To perform the tensile testings, we will be performing continuum simulations using the finite element method(FEM). The sample has multiple notches which are symmetrical in nature and equally spaced along the vertical, Y, axis. All the nodes in X-direction are restrained from moving while a constant strain rate of **2x10-3 s-1** was applied in the Y-direction. The material will follow the constitutive Thamburaja equation which was discussed earlier. Here the almost all parameters were taken from the work of Thamburaja(2011) which represent typical metallic glasses. The elastic constants are taken as G=.7 GPa and κ=.7 GPa. The material constant ζ is taken as 0.02 and ξT pertaining to T=295 K as 0.00063. The parameters s2 and s3 are taken as 2800 and 240 GJ/m3, while fo corresponding to T=395 K is taken as 214.8 s1. Also, in order to seed defect sites and trigger shear bands, Co is perturbed by 1% about its mean value of 1 GPa and randomly assigned to the elements.

2.2.1 Experiment 1 -: In the first case, we have run the FEM simulations on the sample without any notch at the end here the ligament length Bo is taken to be 20nm and the radius of the notch was taken R=10nm and here we have taken another geometric parameter D=40 nm. While we have varied the number of notches and the value of intrinsic length Lc.

(a).Case 1 : Here we will see the effect of varying number of notches or spacing S at the edge while keeping constant all other parameters for intrinsic length Lc=15nm.

(b).Case 2 : In this case, we will see the effect of changing intrinsic length Lc for 6 notches while keeping other parameters constant.

2.2.2 Experiment 2 -: In this case, we have run FEM simulations for continuous notches that is the presence of half notch at the end as well, as we can see in figure 6. The radius of the notch is taken as R=10nm while we have changed different parameters to see the effect of changing their value. We will see the effect of changing ligament length on failure and ductility of nano-metallic glass sample Bo while keeping other parameters constant. In other cases the value of intrinsic length was changed along with this we have run simulations for the sample changing the spacing or the number of notches at the surface for different ligament length while keeping other parameters constant.

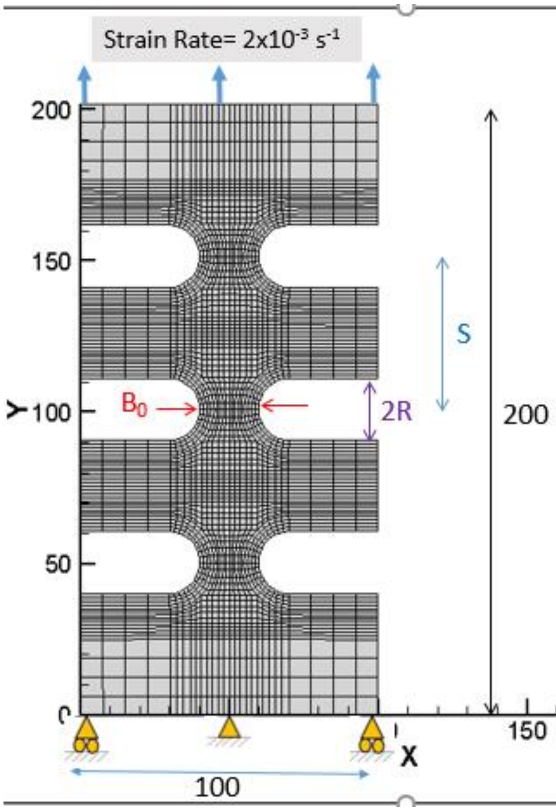


Fig 5:- Aperiodic notches

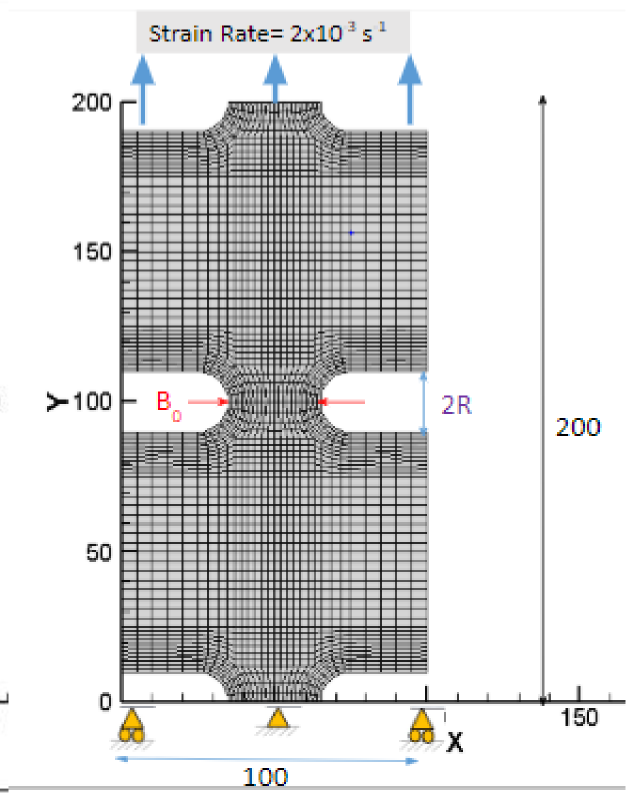


Figure 6:-Periodic notches

Chapter 3. Results and discussion:-

As we have discussed earlier bulk metallic glasses fail catastrophically but when metallic glass sample is taken up to nanometer level the ductility of sample improve rapidly, the sample fails due to shear band formation inside sample, people have shown in experiments that if the sample is rough (roughness ratio-1/20 i.e. notch depth to sample size ratio) or there are presence of notches on the surface of sample fails because of necking. We have conducted continuum finite element analysis of Nano-sized notched MG specimen's behavior on tensile loading.

3.1 Experiment 1: As discussed before the geometric parameters taken here are ligament length B=20nm and radius of notch R=10nm constant, while we have varied intrinsic length and spacing for aperiodic notches.

(a).Case 1:-

Varying spacing between notches for fixed Lc=15 nm:

Stress-strain curve:-

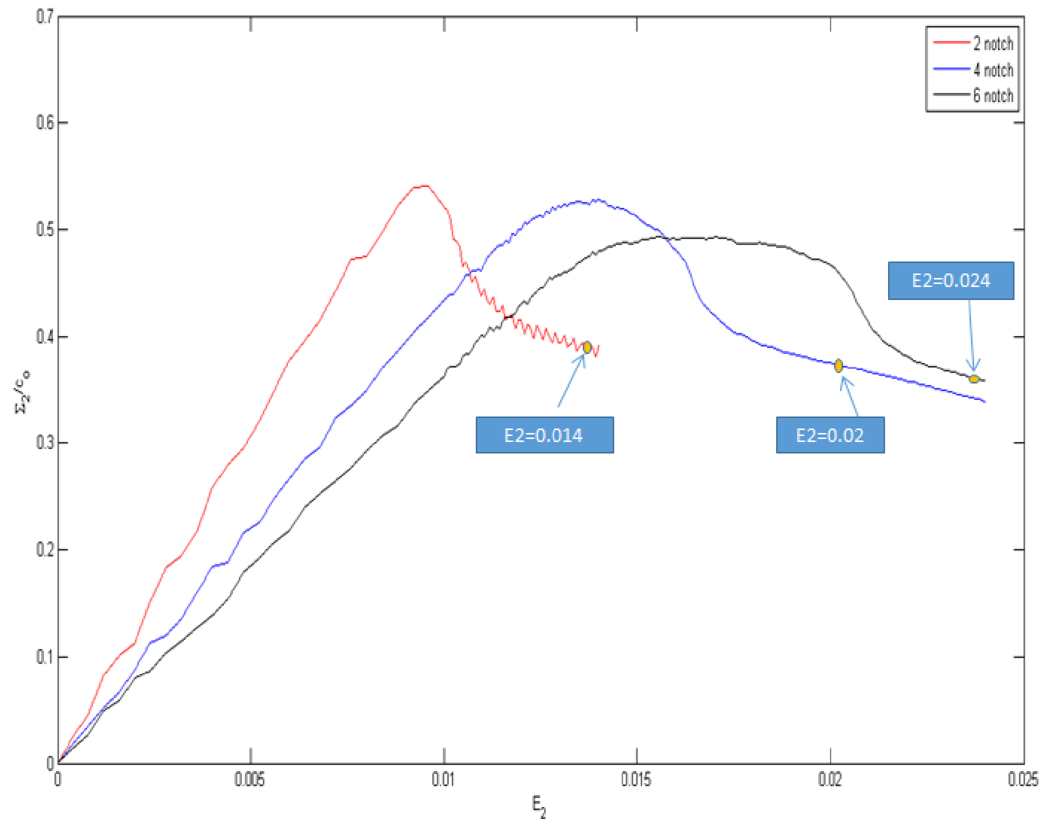
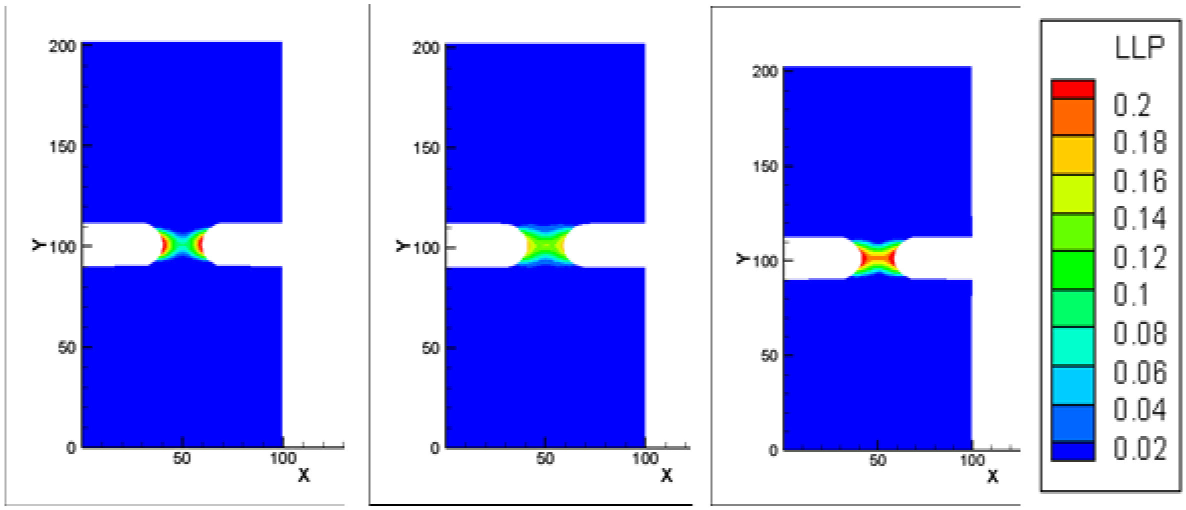


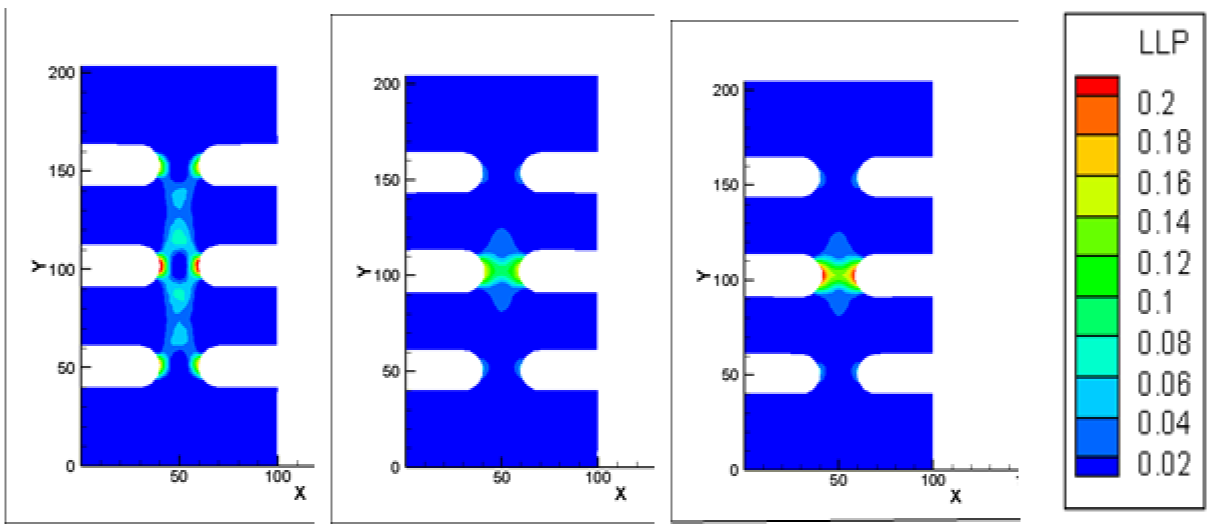
Figure 7- Normalized nominal stress vs strain curve for Lc=15nm for aperiodic notches

Evolution of plastic strain for 2 Notches:



Strain(E)= 0.01 Strain(E)= 0.012 Strain(E)= 0.014

Evolution of plastic strain for 6 notches:



Strain(E)= 0.018 Strain(E)= 0.022 Strain(E)= 0.024

Figure 8- Contour plots of plastic evolution strain inside shear band for 2 and 6 notches for fixed Lc=15 nm of Aperiodically placed notches.

As we can see in the stress-strain curve the strength for 6 notches is low if we compare it with 2 notches this is because more material has been removed but with little loss in strength we get a great improvement in ductility. As we see in the graph after attaining the maximum value of stress the graph suddenly drops due to strain softening for 2 notch sample while in case of 6 notch sample the graph becomes flattered gives a significant amount of plastic strain then drops after formation of the shear band. This large difference in plastic strain for 2 and 6 notch sample is because as the tensile force is applied due to stress concentration shear bands will start forming at the notch tip and then they will propagate inside sample, as there are more number of notches are participating in shear band formation the net effect of applied will be divided amongst notches so the 6 notch sample will give more ductility as compared to 2 notch sample.

(b). Case 2 :-

Varying Lc or intrinsic length for fixed 6-Notch sample:-

Stress-strain curve :

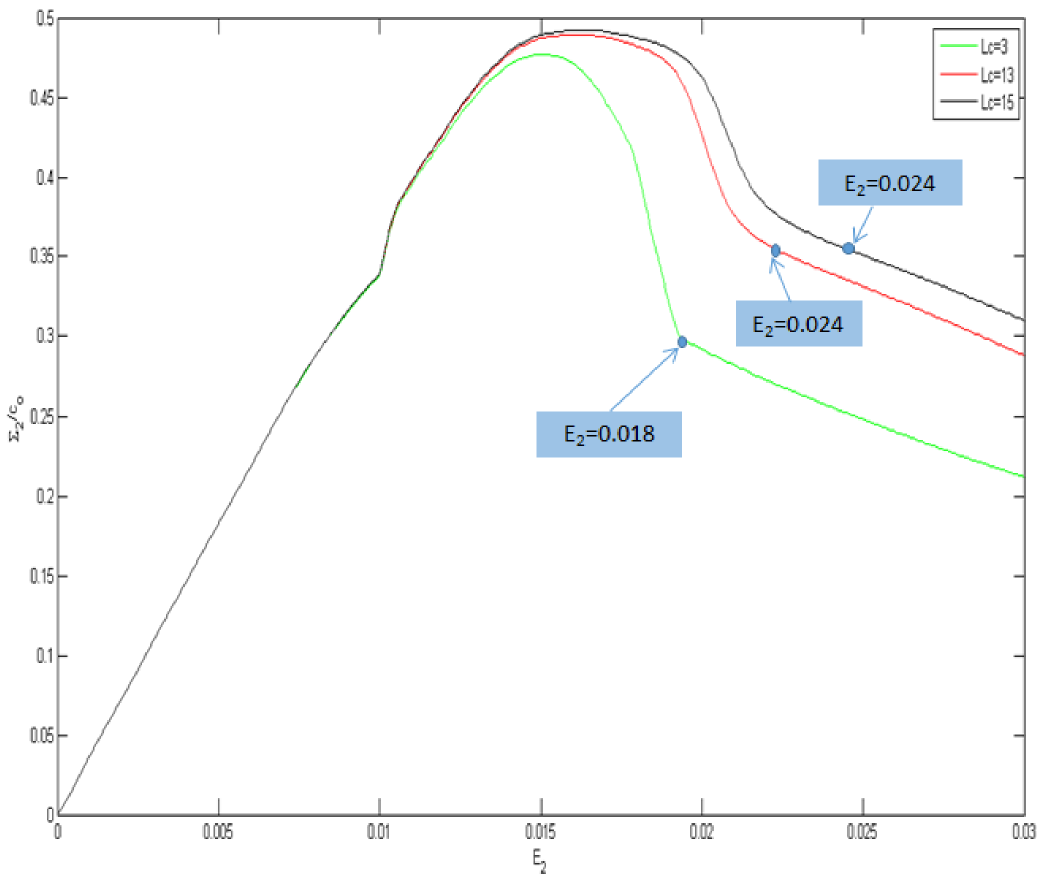
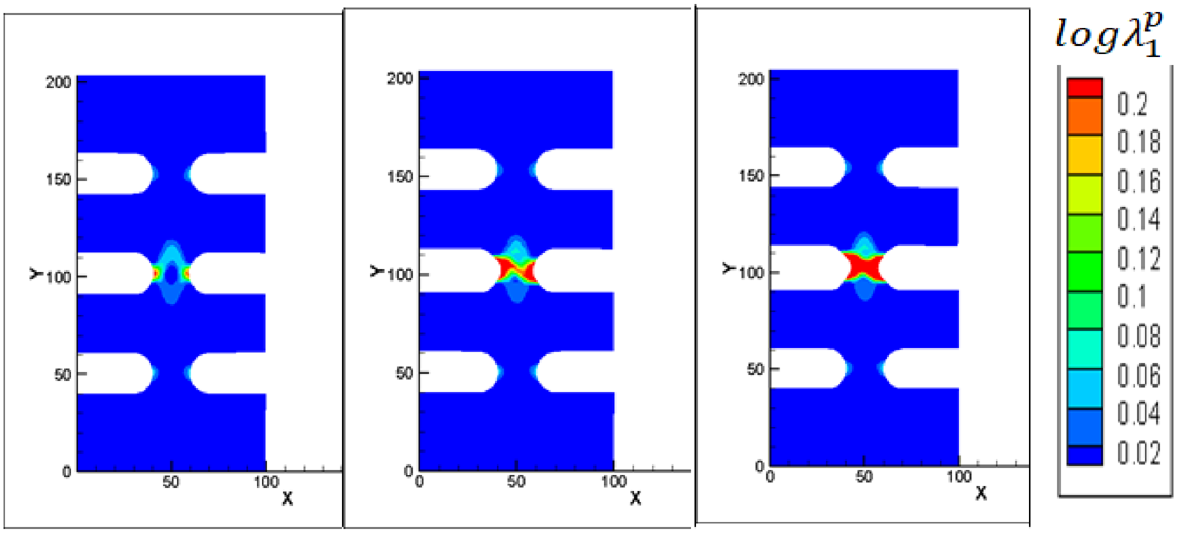


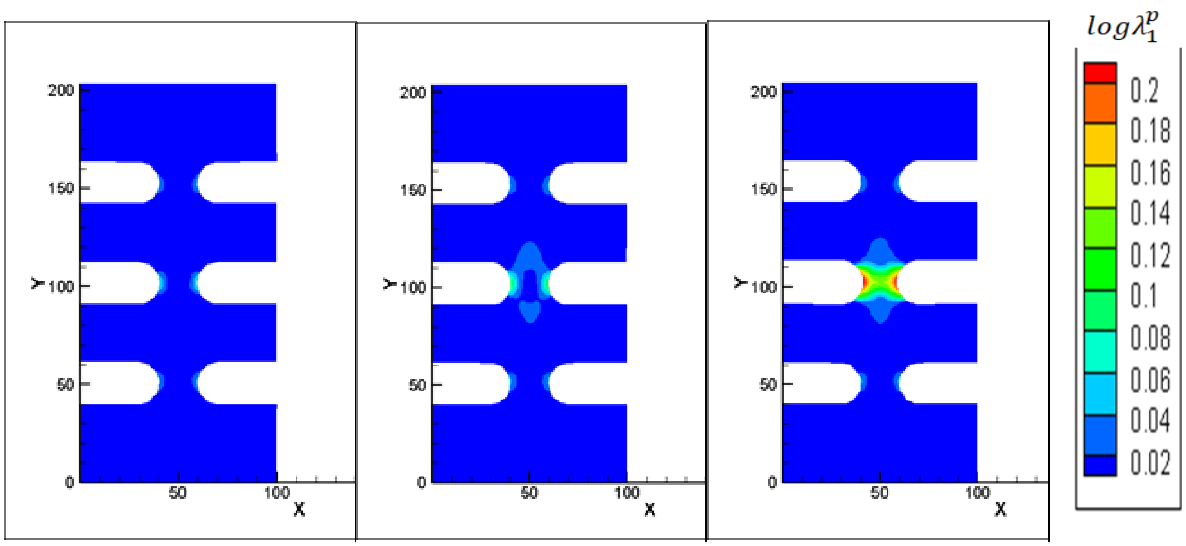
Figure 9- Normalized nominal stress vs strain curve aperiodically placed 6-notch sample

Evolution of plastic strain for Lc= 3nm :-



Strain(E)= 0.018 Strain(E)= 0.020 Strain(E)= 0.024

Evolution of plastic strain for Lc=15nm:-



Strain(E)= 0.018 Strain(E)= 0.020 Strain(E)= 0.024

Figure 10- Contour plots of plastic evolution strain inside shear band for Lc=3nm and Lc=15nm notches for fixed spacing or 6 aperiodically placed notches.

It can be clearly seen from Figure-9 stress-strain curve that when if increase the value of intrinsic length (Lc) the ductility of the sample enhance significantly for applied stress. The contour plots drawn for Lc=3nm and Lc=15nm gives us better idea as the sample for Lc=3nm has already failed before 2.4% strain while the sample with Lc=15nm is not much affected at 2.4% strain as suggested by the value of logλ1p, also for lower value of Lc the sample will fail due to dominant single shear band while for higher value of Lc it will fail due interaction of more than on shear band. The value of intrinsic length is related to the doping of material into metallic glass sample as we vary the composition of materials as width of shear band changes so as we increase the value of Lc the width of shear band increases it means the plastic strain developed into the specimen will be shared by more regions so the ductility will improve.

Contour plots for 6 notches S=50 nm at strain 1.8% for different Lc value.

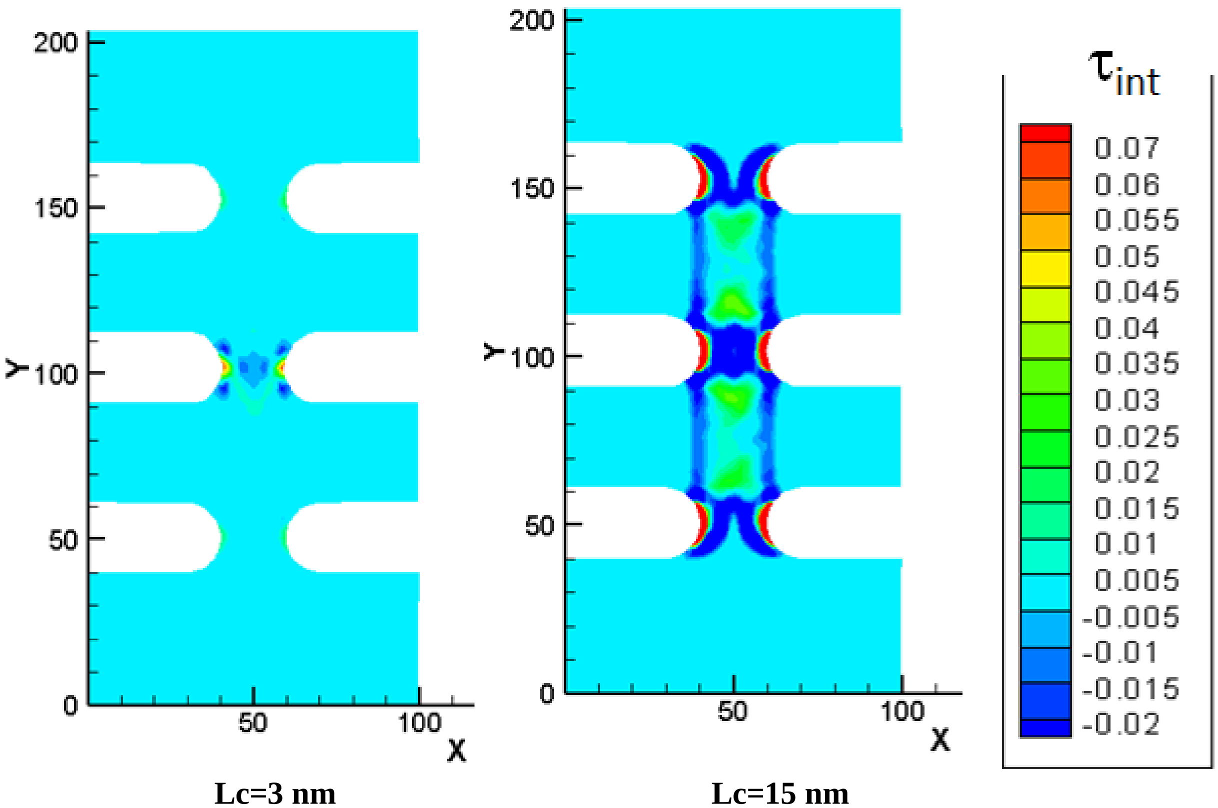


Figure 11- Contour plots for interaction stress (τ int) value inside shear band

In order to understand the role played by the interaction stress on the evolution of plastic strain in the notched MG samples, contour plots of interaction stress, τint, corresponding to two different Lc value for other geometric parameters being constant displayed in figure 11. Plastic yielding commences, thereby causing free volume to evolve (or STZs to accumulate) in front of the notch, at early stage of loading owing to large stress concentration. However, the stress state away from the notch is still elastic. This, in turn, results in a large free volume (or STZ concentration) gradient to develop in front of the notch, and gives rise to interaction stress between the flow defects. A zone of positive-valued interaction stress prevails near the notch root which is circumscribed by a region of negative interaction stress in the form of a semi-circular ring. It must be noted that while positive interaction stress offers resistance to further plastic deformation, negative interaction stress promotes it (see Eq. (b)). Thus, negative-valued interaction stress supports the spread of plastic yielding in a semi-circular region ahead of the notch during initial stage of loading which is seen for Lc 15 nm, So the sample with Lc=15 nm will support more plastic strain in wider region while the sample with Lc=3 nm has already attained the saturation stage of plastic strain on applying further strain will break.

Introduction of periodic notches:-

Comparing between Aperiodic and periodic notched sample for S=50 nm, B=20 nm, and Lc=15 nm.

Stress-Strain curve for Aperiodic and periodic notches :

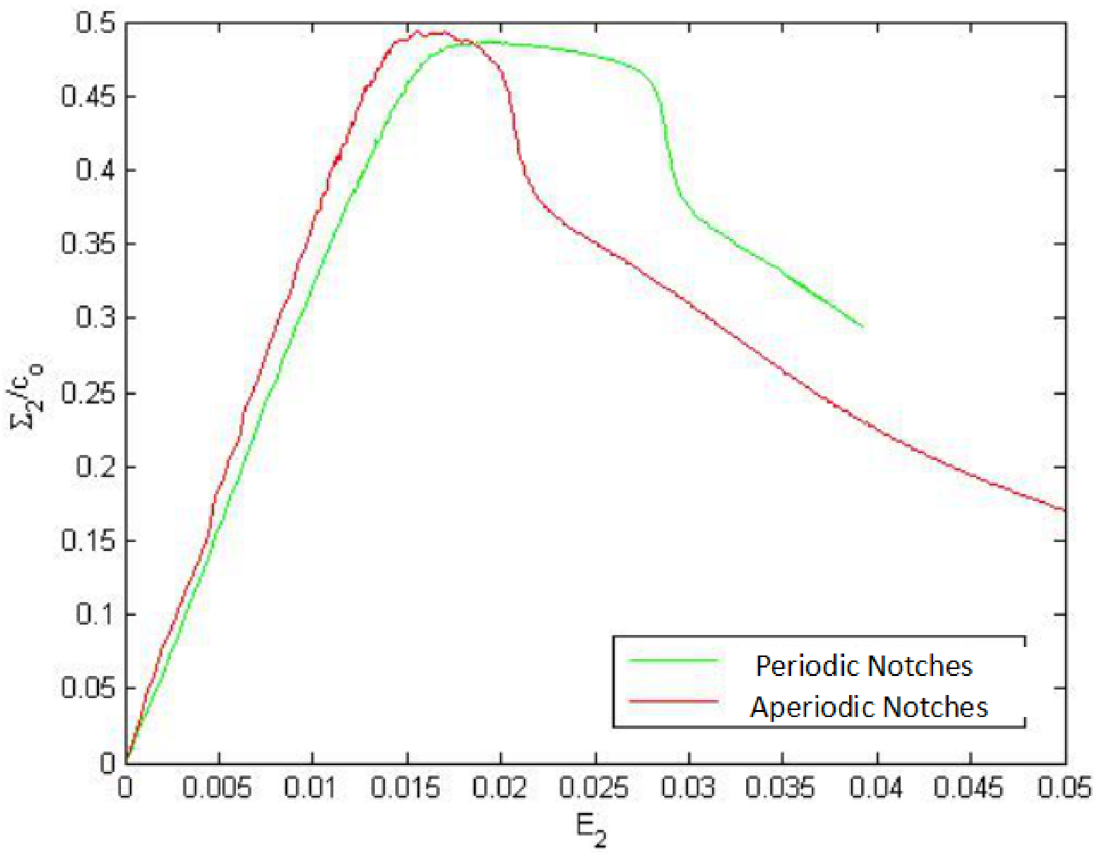
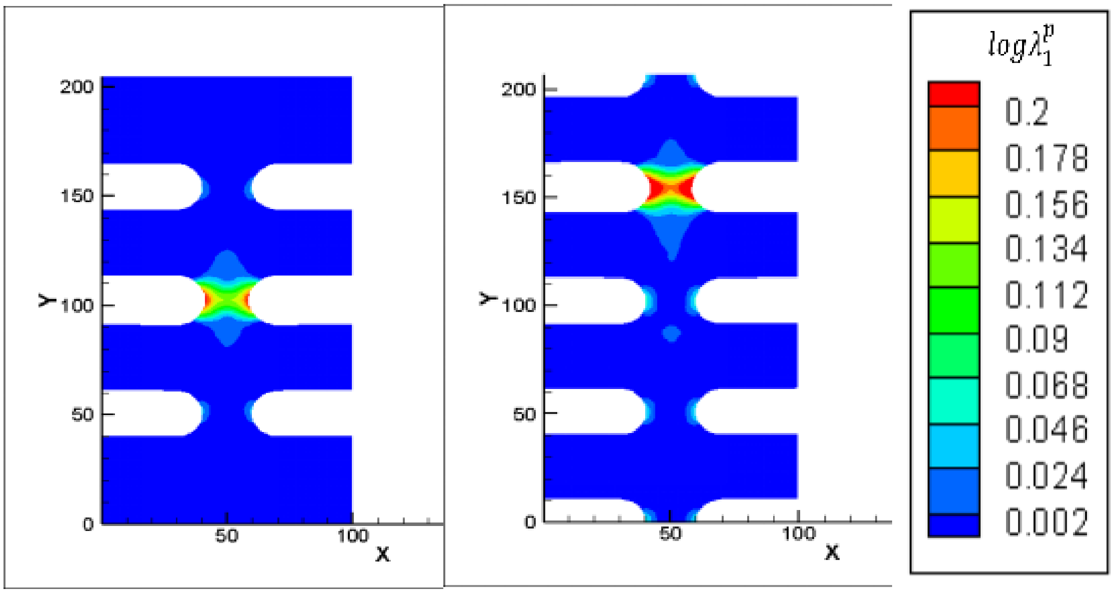


Figure 12- Normalized nominal stress-strain curve for Sample having periodic and aperiodic notches

Contour plots for aperiodic and periodic notches at strain 2.4 % strain for aperiodic notches while at strain 3.5 % strain for Lc=15 nm while other geometric parameters taken as constants



Strain(E)=0.024 **Strain(E)=0.035**

Figure 13:- Contour plots for Aperiodic and periodic notches.

We introduced the periodic notches because in real life the samples will have notches periodically placed across the surface and also we see that the samples with periodic notches will have more ductility see in the (figure 12) as compared to notches placed aperiodically. As we see in the (figure 13) the contour plots the samples having aperiodic notches has failed at strain 2.4% while the sample with periodic notches will fail at strain 3.5%.

<u>3.2 Experiment 2</u> :-

<u>(a).Case 1</u> :-

Varying spacing or number of notches for fixed B=20nm and Lc=30nm.

Stress-strain curve:

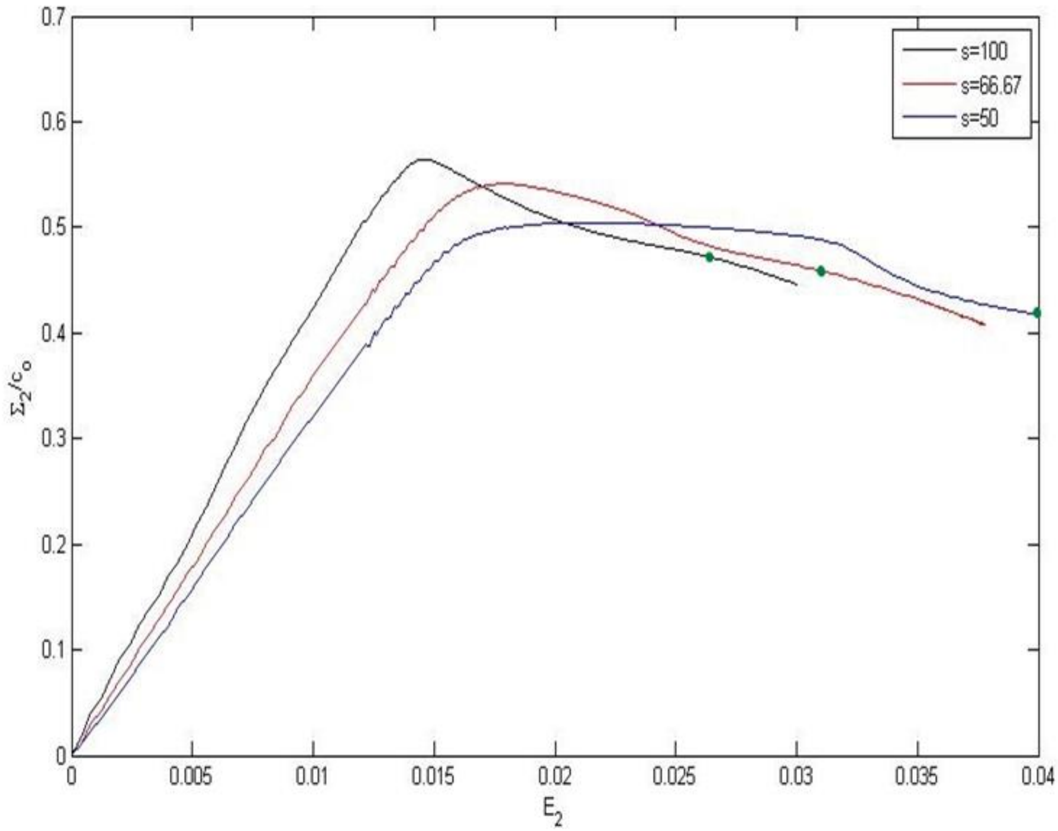
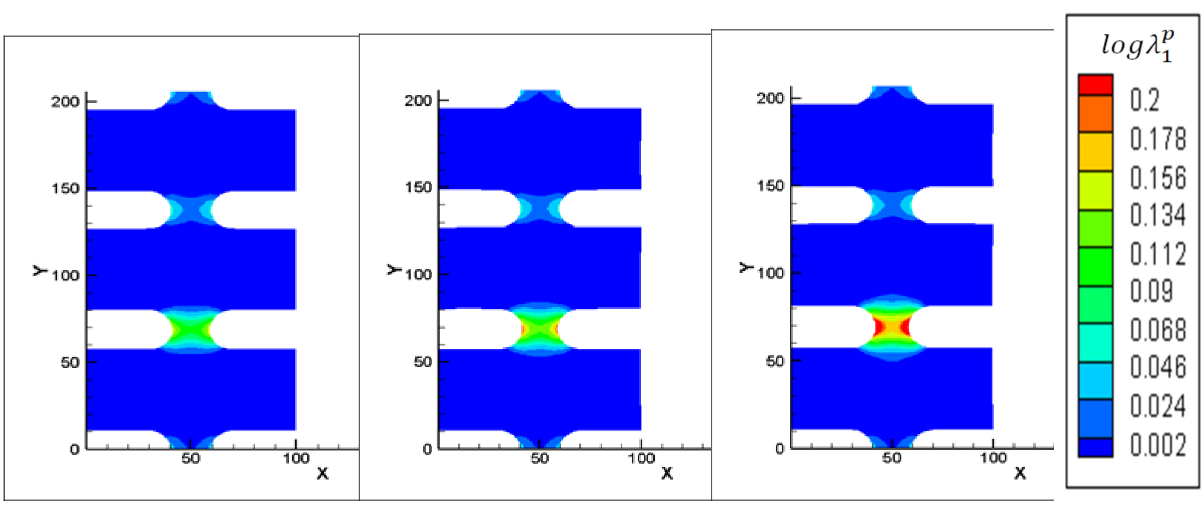


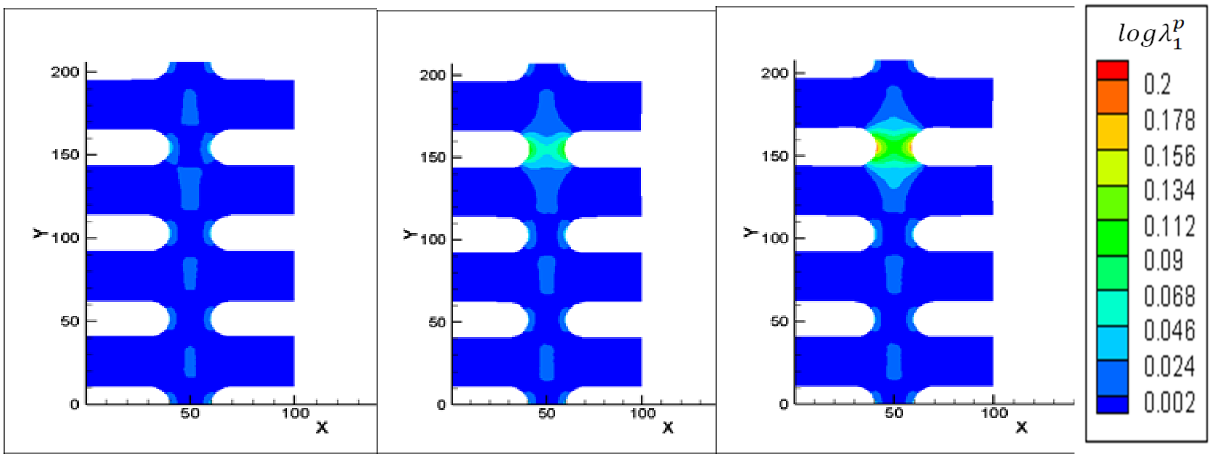
Figure 14-:- Normalized nominal stress-strain curve for sample with Lc=30nm and B=20nm varying spacing between notches

Plastic strain evolution inside shear band for S=66.67 nm :



Strain(E)= 0.028 Strain(E)= 0.030 Strain(E)= 0.035

Evolution of plastic strain inside shear band for S=50 nm :



Strain(E)= 0.030 Strain(E)= 0.035 Strain(E)= 0.040

Figure 15- Contour plots of plastic evolution strain inside shear band for Lc=30 nm, B=20 nm. Varying spacing between periodic notches.

Upon observing the contour plots for different horizontal spacing, we can see that for S=50 nm, the STZs emanating from notch tips interact with each other for a longer period due to presence of more STZs as compared to S= 66.67 nm. Due to longer time taken to interact with each other, S= 66.67 nm shows less ductility by failing at 3.5% strain as compared to S=50 nm which will fail at a strain higher than 4%.

(b). Case 2 : Varying intrinsic length(Lc) for fixed B=20 nm and S=50 nm.

Stress-strain curve :

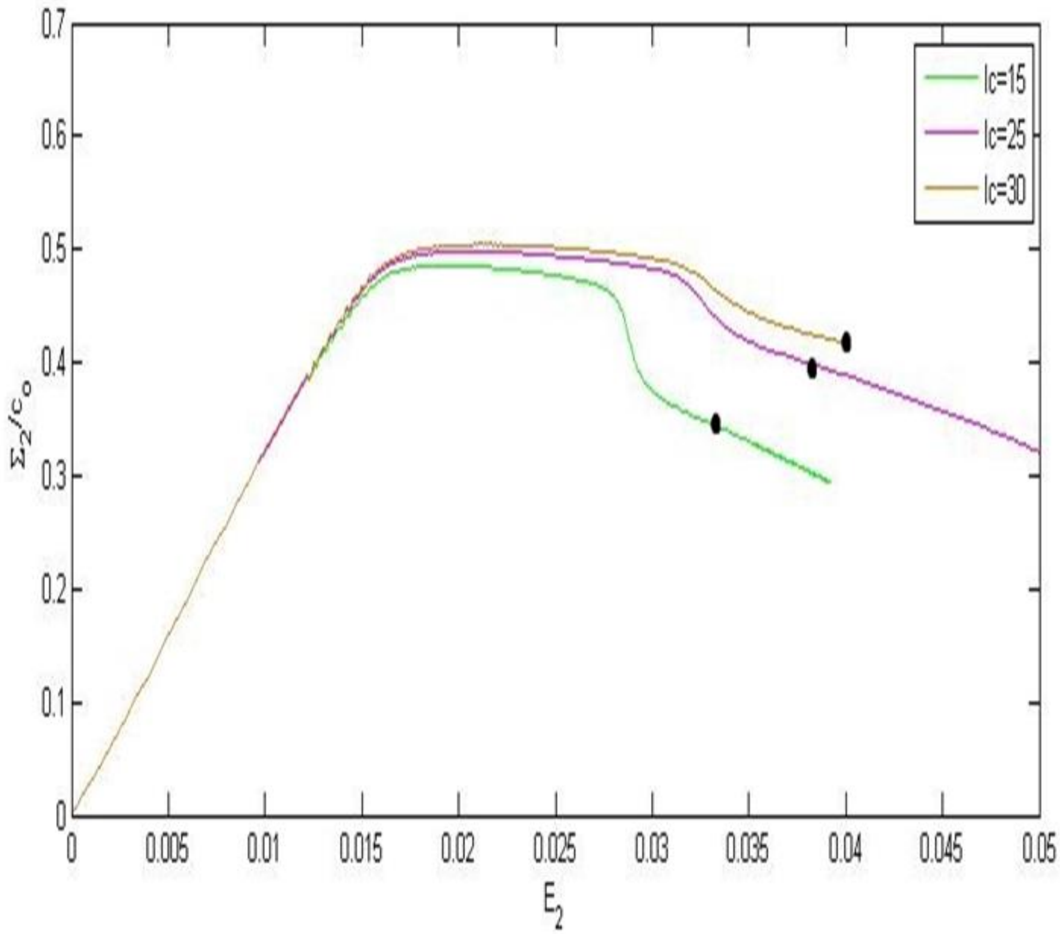
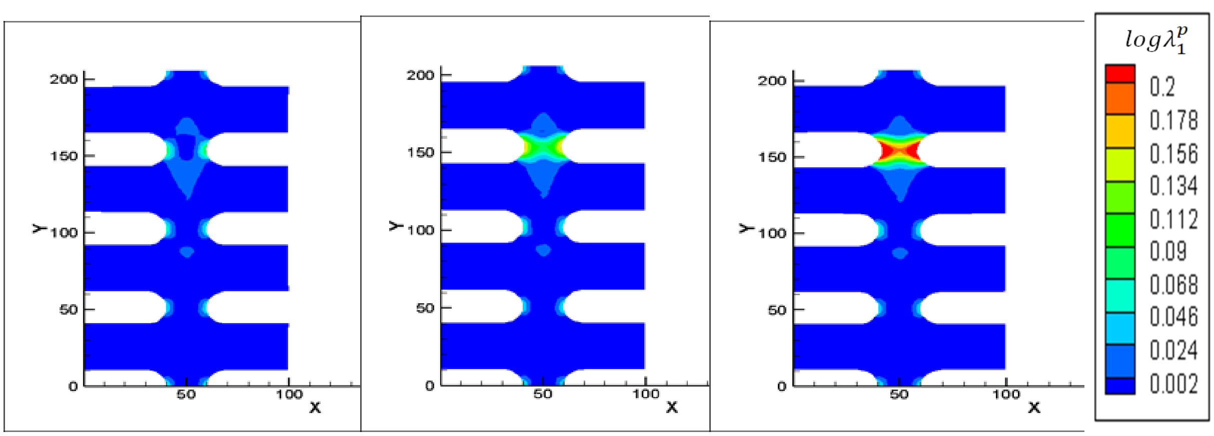


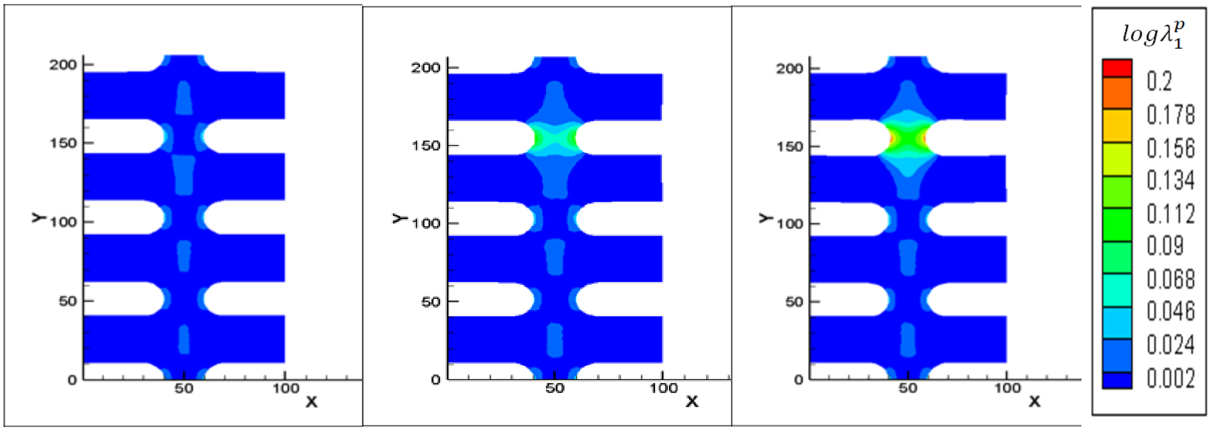
Figure 16-:- Normalized nominal stress-strain curve for sample spacing S =50nm and B=20nm varying intrinsic length value.

Evolution of plastic strain between notches for Lc=15 nm:



Strain(E)= 0.028 Strain(E)= 0.030 Strain(E)= 0.035

Evolution of plastic strain inside shear band for Lc=30 nm:



Strain(E)= 0.030 Strain(E)= 0.035 Strain(E)= 0.040

Figure 17- Contour plots of plastic evolution strain inside shear band for S=50 nm, B=20 nm. Varying intrinsic length.

To understand how much the intrinsic length can be increased so that the ductility keeps on increasing, we increased the Lc from 15 to 30 and made the observation from the contour plots that for Lc=15 nm, the material fails at a strain of 3.5% while there is still no sign of failure in sample with Lc=30. This gives us a result that if the value of Lc is increased further, we can get more ductility as the width of shear band increases and there is increased interaction between STZs which increases the strain when a shear band will be formed.

(c). Case 3 : Varying ligament length(Bo) for fixed S=50 nm and Lc=15 nm

Stress-strain curve:

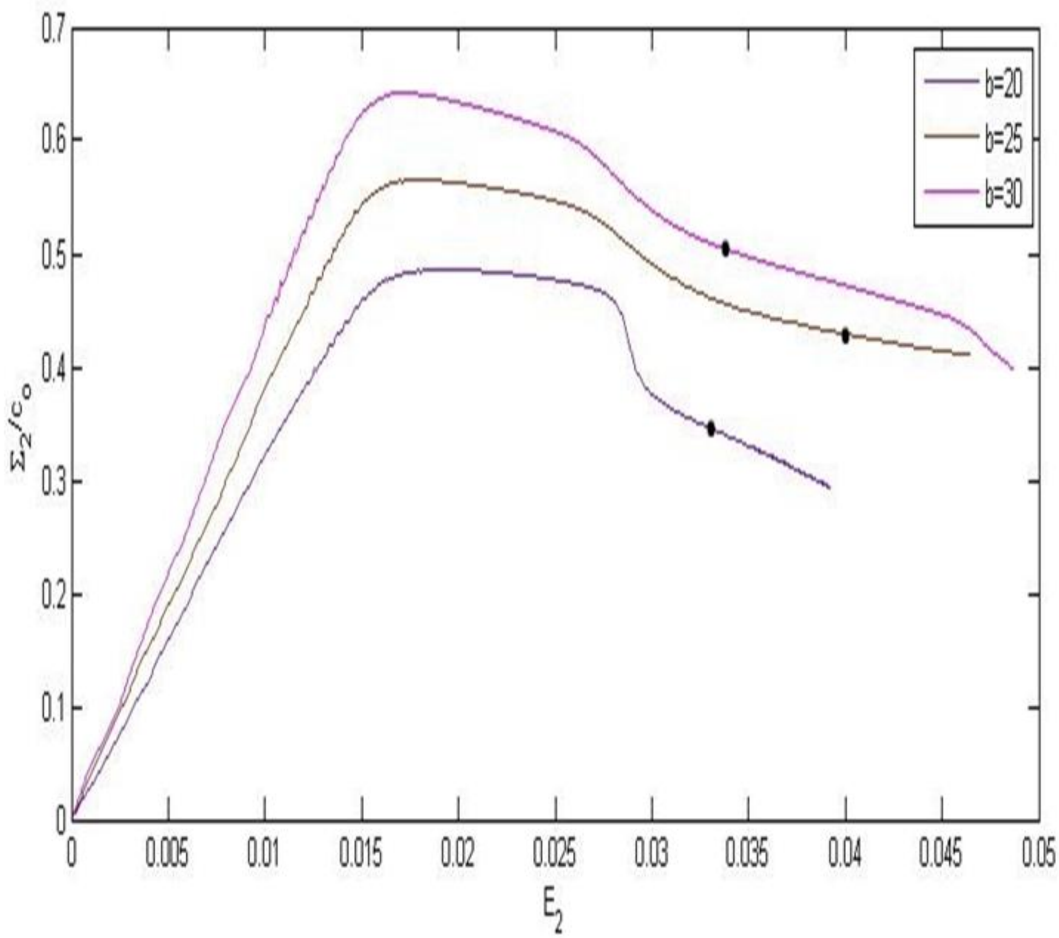
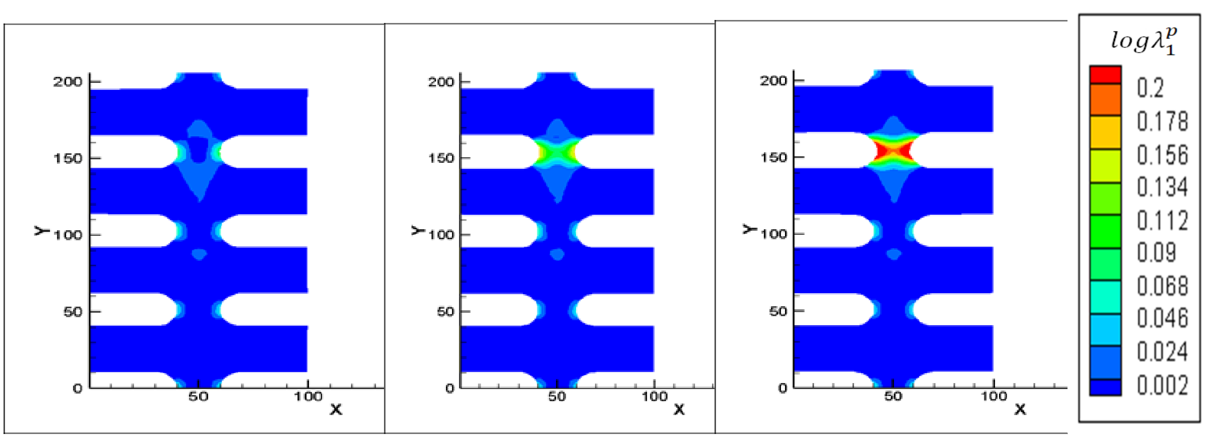


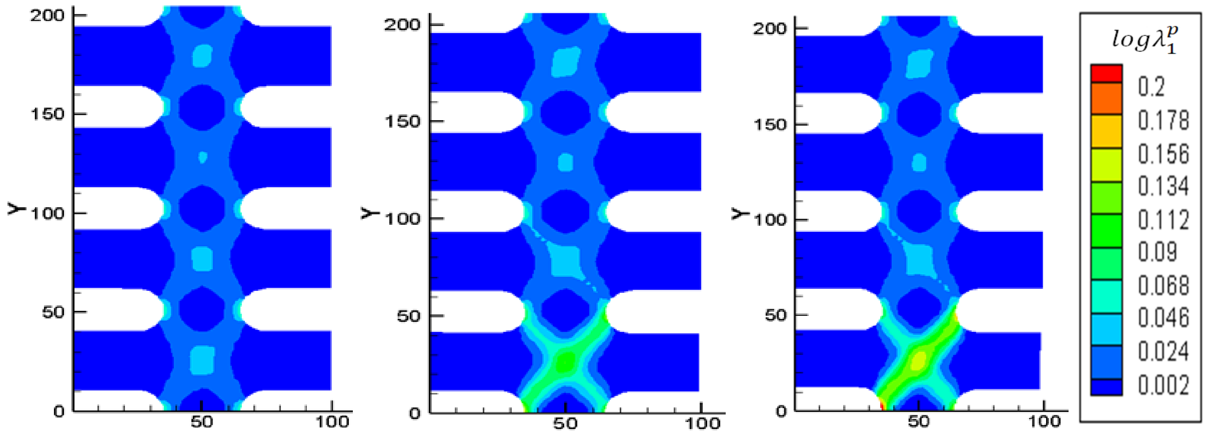
Figure 18-:- Normalized nominal stress-strain curve for sample spacing S =50nm and Lc=15nm varying ligament length value.

Evolution of plastic strain inside shear band for ligament length B=20 nm.



Strain(E)= 0.028 Strain(E)= 0.030 Strain(E)= 0.035

Evolution of plastic strain inside shear band for ligament length B=30 nm



Strain(E)= 0.024 Strain(E)= 0.030 Strain(E)= 0.034

Figure 19- Contour plots of plastic evolution strain inside shear band for S=50 nm, Lc=15 nm. Varying Ligament length.

From the above contour plots we can observe that for B=20 nm, since the notches are close to each other, the STZs interact with each other and are able to form a shear band with the notch opposite to it and undergo necking failure. But for B=30 nm, since the notches are far enough from each other that the STZs are unable to form a shear band with notch opposite to it, rather they form a shear band with the notch diagonally opposite to it and thus failing without necking.

Chapter 4 Conclusion and Future scope:-

4.1 Conclusions

Continuum mechanics simulations were performed on Zr-Cu MG sample of dimension 100 nm x 200 nm to study the effects of changing various parameters in the geometry of the MG sample first in a sample with aperiodic notches followed by periodic notches. After analyzing the stress strain plots and contour plots, we made the following conclusions:

1. Specimens having $2R/B_0=1$ showed necking, whereas specimens having the ratio less than or equal to 0.66 showed failure by forming a dominant shear band.
2. Increasing L_c results in increasing the plastic strain.
3. Decreasing the horizontal spacing between notches increases the interaction between STZs and samples with spacing of 50 nm showed more ductility as compared to samples with spacing of 66.67nm and 100 nm.
4. Introduction of periodic notches increases the ductility (by approx. 1.5%) considerably with almost no compromise in strength of specimen.

4.2 Scope for Future Work

1. Perform simulations on samples with asymmetric notches.
2. Perform simulations on specimens having notches placed in sinusoidal pattern.
3. Perform simulations on specimens with notches having their center outside the sample.
4. Designing specimens with notches having their center on the specimen boundary.
5. Perform similar simulations on specimen having different materials.

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