B. TECH. PROJECT REPORT

On

Finite Element Simulations of Tensile Deformation behavior of Bimodal Nanoglass

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CANDIDATE'S DECLARATION

We hereby declare that the project entitled "Finite Element Simulation of Tensile Deformation Behavior of Bimodal Nanoglass" 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, Associate Professor, Mechanical Engineering, IIT Indore is an authentic work.

Further, I/we declare that I/we have not submitted this work for the award of any other degree elsewhere.

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Dr.Indrasen Singh, Associate Professor, Mechanical Engineering

Preface

This report on "Finite Element Simulations of Tensile deformation behavior of Bimodal Nanoglass" is prepared under the guidance of Dr.Indrasen Singh.

Recent experiments and molecular dynamics simulations have shown that nanoglasses are more ductile that metallic glass while metallic glass possesses higher strength. Due to the low ductility of the metallic glass, it has very few industrial applications. hence nanoglasses came into the picture. To improve the strength of the nanoglass one of the methods given in Molecular Dynamics (MD) simulations is using Bimodal distribution, but the mechanistic reason for this behavior is not clear. In our project, we have done Finite element simulations on various nanoglasses to increase its strength without compromising its ductility. Also, various effects on the stress-strain curves and plastic strain have been discussed with the change in intrinsic material length. we have also included contour plots, graphs and figures to make the report more illustrative.

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<u>Abstract</u>

are a new class of noncrystalline solids. They differ from today's Nanoglasses to their microstructure that resembles the microstructure of glasses due They consist of regions with a melt-quenched glassy structure polycrystals. connected by interfacial regions, the structure of which is characterized (in comparison to the corresponding melt-quenched glass) by (1) a reduced (up to about 10%) density, (2) a reduced (up to about 20%) number of nearest-neighbor atoms and (3) a different electronic structure. Due to their new kind of atomic and electronic structure, the properties of nanoglasses may be modified by (1) controllin the size of the glassy regions (i.e., the volume fraction of the interfacial regions) and/or by varying their chemical composition. (2)Nanoglasses exhibit new properties, e.g., a Fe₉₀Sc₁₀nanoglass is (at 300 K) a strong ferromagnet whereas the corresponding melt-quenched glass is paramagnetic. Moreover, nanoglasses were noted to be more ductile, more biocompatible, and catalytically more active than the corresponding meltquenched glasses. Hence, this new class of noncrystalline materials may open the way to technologies utilizing the new properties. The strength-ductility trade-off has been a common long-standing dilemma in materials science. Our results reveal that large grains impart high strength, which is in striking contrast to the physical origin of the improvement in strength reported in the traditional nanostructured metals/alloys. Furthermore, the mechanical properties of NG with a bimodal nanostructure depend critically upon the fraction of large grains. By increasing the fraction of the large grains, a transition from superplastic flow to failure by shear banding is clearly observed. We expect that these results will be useful in the development of a novel strong and superplastic NG.

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Chapter1. INTRODUCTION

<u>1.1 Amorphous</u> and crystalline solids:

Amorphous solid: 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 defin amorphous solids as materials that don't have a uniform 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: 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-metalli elements (Phosphorus, Sulphur, and iodine).



Crystalline Solid



Amorphous Solid

Figure 1- Arrangement of Atoms



Figure 2-Shape of Crystalline and Amorphous Solids

1.2 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 a combination of various mechanical properties which makes them a suitable candidate for building materials.

Metallic glasses (MGs) have shown attractive mechanical properties such as high strength, yield strain, good corrosion resistance, and substantial fracture toughness. However, they lack ductility under tensile loading and fail catastrophically by crack propagation in a dominant shear band [SB] which is the biggest hindrance for their structural application. This can be achieved by arresting SB propagation and forming multiple distributed SBs, for example, through the addition of crystalline dendrites in the MG matrix. Also, MGs may exhibit homogeneous deformation without SBs when the specimen size is below a critical length scale. Alternatively, global plasticity can be increased by promoting the nucleation of secondary SBs through a priori deformation like cold rolling. The latest advances in the micro/nano-fabrication technology of metallic glasses have aided the potential usage of these materials for integrated circuit applications and also MEMS/NEMS applications such as membrane actuation structures, pressure, and biochemical sensors.

1.3 Nanoglasses

Nanoglasses are a new class of noncrystalline solids. A nanoglass (NG) is a novel architecture that has the potential to tune the properties of metallic glasses (MGs). It consists of nanometer-sized glassy grains separated by the glass–glass interfaces. The atomic structure of these interfaces is similar to individual SBs and is characterized by excess free

volume or low density, lack of short-range order and increase in the concentration of flow defects such as shear transformation zones (STZs). Consequently, the interfaces act as precursors for SB nucleation leading to enhanced global plasticity. Thus, the atomic structure and mechanical response of nano glasses (NGS) are different from MGs.

It is the idea of nanoglasses to generate a new kind of glass that will allow us to modify the defect and/or the chemical microstructures of glasses in a way comparable to the methods that are used today for crystalline materials. The basic concept of this approach is schematically explained by comparing the microstructures of nanoglasses and of nanocrystalline materials. If we consider a melt of identical atoms, we obtain a single crystal if we solidify this melt under conditions close to equilibrium. A nanocrystalline material with a high density of defects in the form of incoherent interfaces is obtained by consolidating nanometer-sized crystals. If the consolidated nanometer-sized crystals have different chemical compositions, e.g., Ag crystals and Fe crystals



Figure 3- Figure showing the analogy between the defect and the chemical microstructures of nanocrystalline materials and nanoglasses. (a) Melt of identical atoms, (b) single crystal. The defect microstructure (c) and chemical microstructure (d) of nanocrystalline materials are compared with the corresponding defect microstructure (g) and the chemical microstructure

(h) of nanoglasses. (f) displays the glassy structure obtained by quenching the melt shown in (e).

The idea behind nanoglasses is to apply an analogous approach, i.e., the consolidation of nanometer-sized glassy clusters in order to generate glasses with a high density of interfaces between adjacent glassy regions with either the same or with different chemical compositions. In other words, by consolidating nanometer-sized glassy clusters (Figure 1g), we generate a solid material that consists of nanometer-sized glassy regions (corresponding to the nanometer-sized crystallites in Figure 1c) connected by interfaces with an enhanced free volume due to the misfit between the atoms at the surfaces of adjacent glassy clusters. Due to the analogy of the nanometer-sized microstructures of both materials (Figure 1c and Figure 1g), the glass shown in Figure 1g is called a nanoglass. Again, if we consolidate nanometer-sized glassy clusters of different chemical compositions (Figure 1h), we obtain a multiphase nanoglass that is microstructurally analogous to the multiphase nanocrystalline material shown in Figure 1d. Hence, this kind of glass is called a multiphase nanoglass.

The idea of nano glasses to generate a new kind of glass that will allow us to modify the defect and/or the chemical microstructures of glasses in a way comparable to the methods that are used today for crystalline materials.

<u>1.4 Production of nano glasses:</u>

1-Inert-gas condensation: One way to produce nanoglasses is by means of inert-gas condensation (Figure 4). This production process involves the following two steps [3-6]. During the first step, nanometer-sized glassy clusters are generated by evaporating (or sputtering) the material in an inert gas atmosphere. The resulting clusters are subsequently consolidated at pressures of up to 5 GPa into a pellet-shaped nanoglass. So far, nanoglasses have been synthesized by inert gas condensation from a variety of alloys: Au–Si, Au–La, Cu–Sc, Fe–Sc, Fe–Si, La–Si, Pd–Si, Ni–Ti, Ni–Zr, Ti–P.



Figure 4- Inert gas condensation process

2-Magnetron sputtering: This method has been applied so far to Au-based metallic glasses The nanoglass obtained consisted of glassy regions with an average size of about 30 nm. Recent studies of the structure and the properties of nano glasses produced by magnetron sputtering suggest that their structure and properties are comparable to the ones of nano glasse produced by inert gas condensation.



Figure 5- Magnetron sputtering process

3-Severe plastic deformation: Due to the enhanced free volume in shear bands the average free volume content of glass was found to increase with increasing plastic deformation. However, despite the similarity between the microstructural features of a nanoglass produced by consolidating nanometer-sized glassy spheres and a nanoglass produced by introducing a high density of shear bands, the results of recent studies by molecular dynamics (MD)and Mössbauer spectroscopy of a ball-milled melt-quenched Fe90Sc10 glassy ribbon and a Fe90Sc10 nanoglass suggest that the atomic structure of both kinds of nanoglass differ. Moreover, the result obtained for an ionic material (LiAlSi2O6) suggests that the microstructure of the ball-milled LiAlSi2O6 glass is similar to the one of the nanocrystalline LiAlSi2O6.

<u>1.5 Applications</u>: Metallic glasses possess high physical and tensile strength and are also resistant to corrosion.

1.5.1: Coating of Metallic Glass:



Figure 6.1- Tools

Figure 6.2- Golfing putter

1.5.2 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 6.3- Pressure sensor

Figure 6.4- Micro gear

1.5.3 Biomedical Industries:(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 implantatio in the human body.



Figure 6.5-Titanium-based BMG alloy tooth implant





<u>1.6 Literature Review:</u> MD simulations of tensile loading have demonstrated that ductility in NGs increases with a decrease in grain size and may eventually lead to superplastic flow for average grain size below a threshold. This has been rationalized on the basis that an the increase in interfaces leads to more homogeneous release of stored elastic energy resulting in the nucleation of multiple, intersecting SBs. While these SBs spread along with the interfaces, they do not connect across the grains to form a contiguous dominant SB when the grain size is sufficiently small. In other words, adequate elastic energy is not available for driving a single dominant SB. However, these studies do not explain the physical origin of the length scale that governs the critical grain size below which no dominant SB forms. Specifically, the following questions arise pertaining to the deformation behavior of NG.

In Molecular Dynamics (MD) simulations (Z. D. Sha et al., 2015, RCS) they have reported that the strength of nanoglass material can be improved by using Bimodal distribution, but the mechanistic reason for this behavior is not clear.

In order to address the above query, tensile loading ofBimodal NGs is analyzed in this work through finite element simulations using a non-local plasticity model\and the effect of grain size and role of interaction stress on ductility enhancement are studied.

Chapter2. FE Modelling

2.1 Generation of bimodal nanoglass samples:

Nanoglass consists of interface and grains. Interface width is around 1-2 nm Free volume of the interface is lower as compared to that of grains. The properties of interface elements are different than the properties of grains.





Here we are using Bimodal Configuration for the FEA analysis of nanoglass. Bimodal Configuration consists of big grains and small grains. The size of the big is around 3 times the size of the small grain. bimodal nanoglass are generated using NEPER (polycrystal generation and meshing) software. The equivalent diameter of the big and small grains is given as input to generate the required bimodal samples.

2.2 Meshing of bimodal nanoglass:

The meshing of Bimodal nanoglass is difficult to be done by standard meshing software due to its irregularity in grain size and also due to the interface that exists between the boundary of grain domains. Here the NEPER software is used for the meshing of nanoglasses. It can deal with 2D and 3D polycrystals with very large numbers of grains. Meshing involves specific methods called regularization, multimeshing, and remeshing. The mesh size can be uniform or defined on a per-grain basis. Meshing with cohesive elements at interfaces. Visualization and analysis of the tessellations and meshes can be done. In Neper, tessellations can be generated using size or equivalent diameter of grains. For the generation of Bimodal NG values of small and big grains are given as input. NEPERalso generates images of Tessellation and Mesh in png format.



Figure 9- Meshing through NEPER

2.3 Collecting Interface elements through Algorithm:

As the interface elements have different properties than that of interior elements, it is necessary to segregate the elements on the interface and interior of grains. There is No standard software that will segregate the elements, not even NEPER is capable of this. So we came up with an Algorithm to distinguish the elements in interface and grains. In this algorithm, we are reading the image generated through NEPERusing OpenCV. Here is the Block Diagram of the Algorithm for getting Interface elements.



Figure 10- Block Diagram of Algorithm







Interface elements

Image generated through NEPER

Mesh Image

Figure 11- Interface elements collection

In the above algorithm, the interface width was taken to be around 2 nm so as covering 4 interface elements. But then to further increase the efficiency the interface width was taken to be around 1nm i.e. covering 2 elements in the interface.

<u>2.4 Constitutive Model</u>

To perform the simulations, we will be using the model proposed by P. 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.

2.4.1 Interaction stress, Cint: For understanding this let's consider an example of a wire carrying electric current. This wire has a magnetic field around it that 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 a 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.

2.4.2 Intrinsic Material Length, L_c: Infinite element simulations, we don't have a direct method of controlling the composition of the specimen. Therefore we use another parameter that can capture this effect. The intrinsic material length is responsible for controlling the width of the shear band and is short ordered of few nanometers, i.e., it plays a significant role when the specimen is on the 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 a few basic definitions, we can proceed with understanding how free volume generation happens in the shear bands.

$$\dot{\xi} = \dot{\xi}_0 \left(\frac{s_1}{s_3}\right) \left(\nabla^2 \xi\right) + \zeta \dot{\gamma}_p - \left(\frac{\dot{\xi}_0 \bar{p}}{s_3}\right) - \dot{\xi}_0 \left(\frac{s_2}{s_3}\right) \left(\xi - \xi_T\right) \tag{1}$$

$$\dot{\gamma} = \begin{cases} \dot{\gamma_o} \left(\frac{f}{c}\right)^{\frac{1}{a}} f = (\overline{\tau} - \tau_{int} - \zeta(s_2(\xi - \xi_T) + \overline{p}) > 0 \quad Where \ \tau_{int} = -\zeta s_1 \nabla^2 \xi \ (2) \\ 0 \quad f \leq 0 \end{cases}$$

I-Free Volume Diffusion

When amorphous metals are subjected to any stress, then the free volume diffuses throughout the specimen. This diffusion of the free volume is dependent on the temperature of the specimen and thus thi behavior 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 the shear band is controlled, then plastic strain develops in this region.

$$L_{c} = \sqrt{s_{1}/c_{o}}$$
(c)

From equations (a) and (b), we can observe interaction stress is dependent on intrinsic material length, L_c . 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 collapsing together and forming shear bands in those regions.

2.5 Modelling Aspects:



A rectangular specimen (48(W)*96(L))nm has meshed with quad type mesh elements. The size of the mesh elements is 0.6 nm. The bimodal sample has small grains and large grains whose size is approximately 3 times of smaller grains. The size of the small grains is kept constant throughout the experiments which are 6 nm while the size of the large grains has been selected to get appropriate results. All the nodes in X-direction are restrained from moving while a constant strain rate of **2x10-3s-1** was applied in the Y-direction. The material will follow the constitutive Thamburaja equation which was discussed earlier. The material Property for the above FE Model is-

2.6.1-Property for the elements in the grains:

k=166.7 Gpa	G=35.7 Gpa	ζ=0.02	S ₂ =2800GJ/m^3
S ₃ =240GJ/m^3	$\gamma_0 = 1.73 * 10^{(-3)}/S$	a=0.02	ф=0.076
K=-250	$\xi_{T} = 0.00063$	$f_0 = 214.8 S^{\Lambda(-1)}$	C ₀ =1 Gpa for MG

2.6.2-Property for Interface elements: All values are same except: $K = -100, C_0 = 0.8$ Gpa

Chapter 3. Results and discussion

On running various simulations by changing the number of small grains and large grains thus changing the total number of grains keeping the size of small grain as 6nm and large grain as 12nm constant, it was observed that the significant rise in the peak of the stress-strain curve was shown by two models. The Bimodal configuration with 10 large grains and with 15 large grains showed a significant rise. So further studies of parametres are done on these two configurations. Before that, we made some simulations to check our results are in accordance with MD simulations results.



fig 13. and fig 14. -Comparison of our FEA results with molecular dynamic simulations results

In the above image of the stress-strain curve, the Bimodal NG curve is shown by the black color. Stage 1 is the elastic region, stage 2 is in the plastic region where the formation of the shear band starts, stage 3 and 4 are in the phase where the shear band gets saturated this behavior of curves can be understood better by the contour plots.



Figure 15 - Contour plots of maximum Logarithmic plastic strain at different strains

<u>3.1-Effect of Interface Width:</u> The number of large grain in this Bimodal Configuration is 10 with an average size of 19nm. The number of small grains is 50 with average small grain size is 6nm interface width lies between 1.2-1.8 nm and area fraction interface is 0.184.



(a) Bimodal Configuration (b) Interface width 1.8nm(c) Interface width 1.2nmFig 16-Configuration with 10 large grains



Figure 17- Normalized nominal stress vs strain curve for Lc=8nm showing interface width effect for 10 grains

As observed from the stress-strain curves the rise in the Bimodal graph is more for less interface width as compared to sample with an interface width of around 1.8nm. The rise in peak is 3%. Some similar trend is observed when the Bimodal configuration is changed. IN the changed configuration the number of larger grains is 15 with an average size of nm and the number of small grains is with an average size of nm.



(a)Bimodal Configuration

(b) Interface width of 1.8nm (c) Interface width of 1.5nm **Fig 18**-Configuration with 15 large grains



Figure 19- Normalized nominal stress vs strain curve for Lc=8nm showing interface width effect for15 grains

3.2 Effect of Intrinsic Material Length: Intrinsic Material Length is an internal parameter depending on the composition of the material and size of the component.

$$L_c = \sqrt{s_1/c_o}$$

1.6

Where s_1 is resistance to plastic deformation and c_0 is initial cohesion which is resistance to plastic yielding or simply shear strength of the material. Here we have taken lc values as 8,15,20. Here the material length effect is seen on Bimodal 10 and 15 configurations. From the curves, it is observed that as the lc values increase the drop in the graph is slow. Reason can be explained through the contour plots







Figure 21- Normalized nominal Stress-Strain Comparison for different lc values for 10 and 15 large grains

Contour plot of maximum logarithmic plastic strain $(Log\lambda_1^p)$

1- Configuration 1 (10 large grains)



Figure 22- Contour plots of maximum logarithmic plastic strain forConfiguration 1 at a plastic strain $E_2=0.04$ for 10 large grains

2- Configuration 1 (15 large grains)



Figure 23-Contour plots of maximum logarithmic plastic strain forConfiguration 1 at a plastic strain $E_2=0.04$ for 15 large grains

As observed from the contour plots as we increase the strain, the shear band formation begins and slowly it grows in magnitude and thickness with rising strain levels. Until the dominant shear band forms the depict permanent failure of the sample. Also observed from the contour plots of logarithmic plastic strain that the maximum plastic strain occurs at the center of the shear band which is depicted by the dark red color. As we move away from the center of the shear band the magnitude of the plastic strain decreases. Also at higher lc, the magnitude of maximum strain is less than that at lower lc. With the increase in lc formation of shear band delays and its width increases which is depicted by the light green and yellow colors on the shear band of lc15 and lc20 samples.

Here we have calculated the shear band width at different strain points for different lc values.

3.3 Variation of logarithmic plastic strain ($Log\lambda_1^p$) in the shear band:



3.3.1: Configuration 1 (10 large grains)

Figure 24- Shear band width comparison for different lc values for 10 large grains



3.3.2: Configuration 1 (15 large grains)

Figure 25- Shear band width comparison for different lc values for 15 large grains The sheer bandwidth is around 1.5-2 nm for 10 large grain configuration and for 15 large grain configuration, the shear bandwidth is around 2-3 nm. So it can be observed that with the increase

in lc values the log values decrease.



<u>3.4 Effect of interaction stress (τ_{int}) for different values of lc</u>

Figure 26 Contour plot of interaction stress (τ_{int}) for different values of lc at E₂=0.015

This can be explained by the Contour plot of interaction stress for different lc.

At a strain of 1.5% just after yielding after the beginning of the development of interaction stresses. This happens due to interaction stresses formed in the sample. As lc of the samples is increased from 8nm to 20 nm, negative interaction stresses are formed in the grain depicted by the blue color while positive interaction stresses are formed in the interfaces depicted by the blue color. Negative interaction stresses formed in the grain promote further plastic deformation while positive interaction stresses formed in the interfaces resist the plastic deformation thereby delaying the formation of the shear band.

This can be mathematically explained by the constitutive equations given above in the constitutive model.

Negative interaction stresses increase the driving force and driving force is directly proportional

to plastic strain increases the deformation.

While positive interaction stresses formed in the interfaces lowers the driving force thereby decreasing the plastic stain and resisting the plastic deformation.

3.5-Configuration effect:

To show the stochastic effects of size and spatial distributions of grains in the samples, our simulations are repeated for a set of different samples with the same number fraction of large grains Here we tried to change the position of large and small grains i.e the orientation is changed. The sample-to-sample variations in stress-strain curves are found to be insignificant. The stress-strain curves are the same for all configurations for different values of lc. The results are in accordance with the MD results.

3.5.1-Number of large grains is 10:







Figure 28- Curve comparison of different lc values of configurations with 10 large grains



3.5.2-Number of large grains is 15-

Figure 29- Different Configuration of 10 large grains

Stress Strain Curves-



Figure 30- Curve comparison of different lc values of configurations with 15 large grains

In summary, the FEA of NG with bimodal grain size distributions has been performed. At no ductility tradeoff, a modest but relevant improvement in the strength is observed in NG with a bimodal grain size nanostructure. Our results reveal that the large grains are responsible for the strength enhancement observed, which is in striking contrast to the physical origin of the improvement in strength reported in the traditional nanostructure metals/ alloys. Furthermore, the mechanical response of NG with a bimodal nanostructure is found to be strongly dependent on the fraction of large grains. On increasing the fraction of large grains, a transition in deformation mode from superplasticity to shear banding is observed. Our results provide not only an in-depth atomic understanding of the mechanical properties and deformation mechanism of NG with a bimodal grain size distribution but also propose an effective way to attain superior mechanical properties of NG through the use of grain size distributions as a design parameter.

Chapter 4. Conclusion and Future scope:

4.1 Conclusions:

Finite element simulation of bimodal nanoglass for tensile deformation was performed and change in deformation mechanism was studied by changing the lc i.e. intrinsic material length on the various configuration of 10 and 15 large grains. After analyzing the stress-strain plots and contour plots, we made the following conclusions:

- 1. Rise in the strength of nanoglass without compromising ductility has been achieved for both 10 and 15 large bimodal nanoglass configurations.
- 2. As we increased lc from 8nm to 20 nm there was a delay in the formation of shear band i.e. with an increase in lc formation of shear band delays.
- 3. Shear band width enhances with an increase in lc.
- 4. Change in the position of grains does not change the deformation mechanism.

4.2 Scope for Future Work

1. Perform simulations on samples with regular grain shapes

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