Finite Element Analysis of Effect of Reinforcing Fillers on Mechanical Properties of Composites and Crack Propagation

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ABSTRACT

In this progressing world, materials are being developed on the basis of their reliability and durability. Composites have made their way out of many engineering materials to stand next to steel in terms of industrial usage and applications which have paved channel for the researchers to work on composites.

This study encapsulates the effect of different filler concentration on the tensile strength of nano-composites. Silica has been used as reinforcement filler and polymer as the base material. Representative volume element (RVE) of various concentrations have been used and effect of filler concentration on tensile strength have been studied. RVEs with different percentages of filler materials 1%, 5%, 10%, 15% and 20% are generated in Digimat and imported to Abaqus to carry out further study.

With increase in filler concentration, there is a trend that the composite material is following which is well demonstrated in their stress-strain graph. With perfectly bonded condition, the trend shows an increase in the ultimate tensile strength. However, when we applied loosely bonded condition on the filler material and matrix; a decrease in ultimate tensile strength was observed. The softwares that are used to carry out this study are Digimat and Abaqus. The crack propagation on these composites with spherical inclusions is conducted in the XFEM (extended finite element method) of Abaqus.

Keywords: Crack propagation, filler concentration, silica, poly

TABLE OF CONTENT

TABLE OF FIGURES

TABLE OF TABLES

CHAPTER 1: INTRODUCTION

1.1 Motivation and Scope

Research on composites has been driven by the necessity to develop materials with improved properties, increased durability, and reduced weight for various applications. The field continues to advance as new materials, manufacturing methods, and technologies are developed, leading to a wide range of applications in diverse industries. In modern times, studies around composites are majorly focused on how to optimize them for certain specific applications. Tensile strength is one of the major mechanical properties of any material which can diversify the horizon of its usage. This particular attribute was the driving force of the study that is conducted in this thesis.

Studying crack propagation is a critical aspect of engineering and materials science with broad implications across various industries and disciplines. This study provides a better command over integrity of structure, strength of material and generic material behavior especially in the aspect of safety considerations. When epoxy-silica composites are in context, the presence of silica as particles must interfere with the pathway of the crack and thus, contributing in overall material strength.

1.2 Aims and Objectives

The ultimate aim of this thesis is to explore the mechanical properties of epoxy-silica composite at different filler concentrations in order to explore different utilities of these composites. Three objectives defined that are to be achieved in the following work are:

1.2.1 Develop numerical model of the effect of filler concentration on tensile strength of particulate composites

Theoretically the percentage of filler material effect the properties of composite material so to inspect how it affects tensile strength specifically is what is studied in this thesis. A numerical model is also incorporated within. We have altered the filler concentration by 1%, 5%, 10%, 15% and 20% respectively and studied the effect on tensile strength graphically.

1.2.2 Generate stress-strain graph of the particulate composites

To determine tensile strength, we generated stress strain graph of each of the distinctive composite with a different filler concentration. This enhanced the effect the filler concentration was having on the composite as a whole.

1.2.3 Develop numerical model of the effect of filler on crack propagation of particulate composites

Crack propagation plays an important role to determine material failure. Such study helps in utilizing the material accordingly and aids develop methods which can help strengthening of the material. We have conducted simulation in which we can trace crack propagation in the epoxy-silica composite at a certain filler concentration.

1.3 Research Methodology

The research methodology to carry out this thesis is illustrated in the following flow chart.

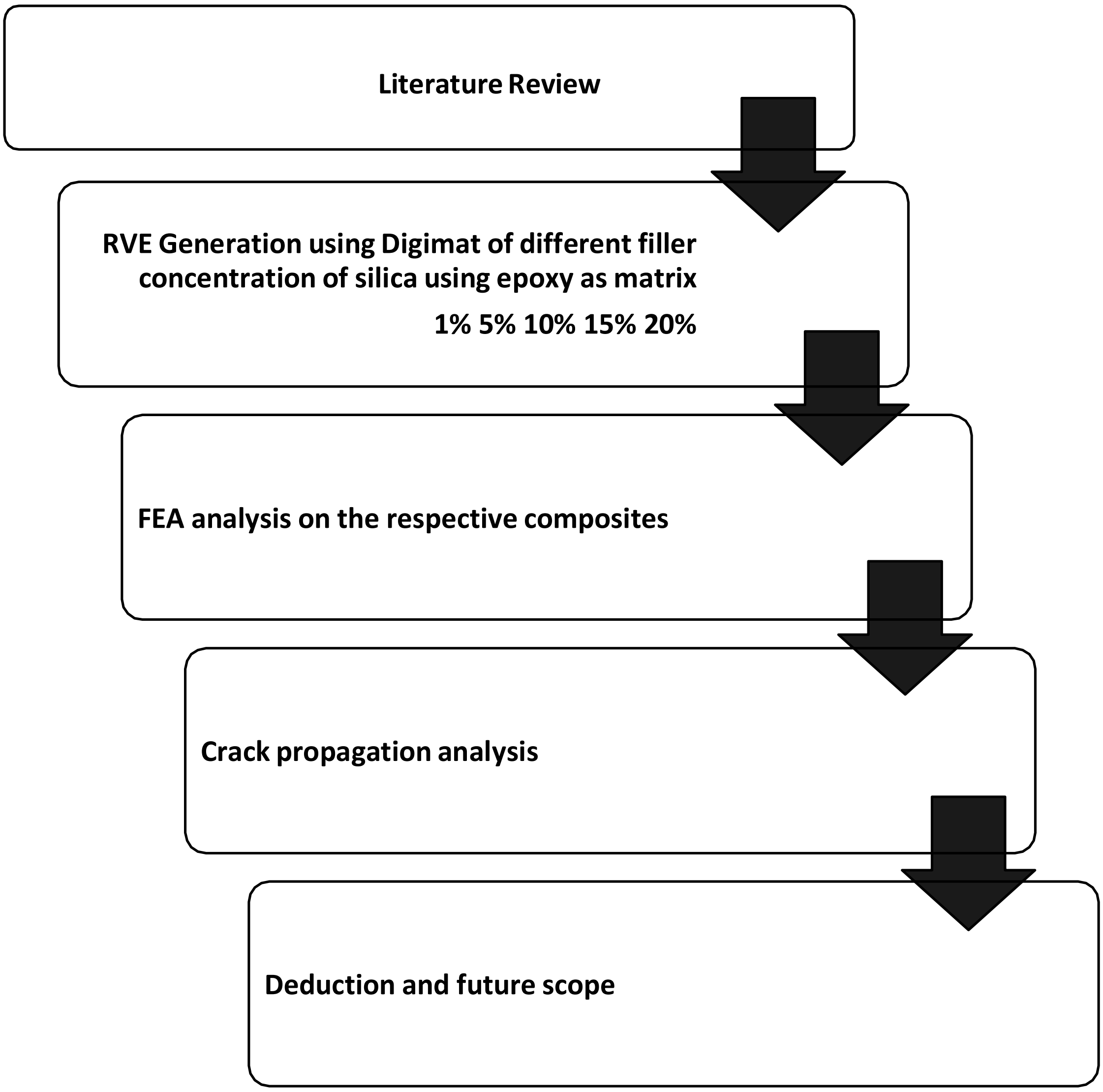


Figure 1 Flow Chart of research methodology

CHAPTER 2: LITERATURE REVIEW

2.1 Composites

Composites are composed of two or more different materials having different physical and chemical properties to bring about a different material possessing different set of properties as per the requirement [1]. Due to their various known properties discussed in upcoming chapter, composites have always grabbed the attention of researchers.

The composites are constituted of two major components namely:

i. *Matrix*- The matrix of a composite holds the reinforcement material in place. It is basically a continuous phase which provides strength to the structure.

ii. *Reinforcement Material*- The discontinuous phase embedded within the matrix is known as the reinforcement material [2]

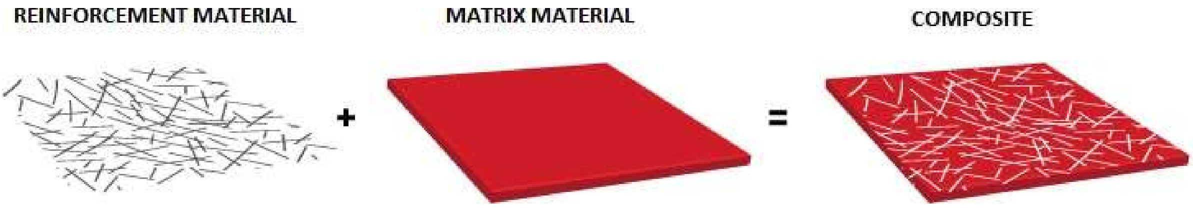


Figure 2general structure of composites

2.1.1 Types of Composites

Due to different structures of the reinforcement materials, and different matrix and reinforcement materials, composites are widely classified in the following categories:

i. Fibre reinforced composites- Composites having continuous fibres embedded in matrix material. Fibre reinforced composites are usually utilized in structural components to reduce weight specifically in the transportation sector since fibre reinforced composites are high-strength lightweight materials, which have highly specific mechanical properties versus regular materials used in construction, such as aluminum or steel. [3]

ii. Particle reinforced composites- Composites in which particles are suspended within the matrix. Particle reinforced composites achieve lower strength and are more cost-effective than other types of composites hence it has applications in consumer products where a balance between performance and cost is important.

iii. Laminar composites – Composites which have different layers of materials binded in a matrix. Laminar composites exhibit high strength to weight ratio and anisotropic properties to achieve different mechanical characteristics in different directions. This can be advantageous for specialized applications for aerospace, automotive and marine industries.

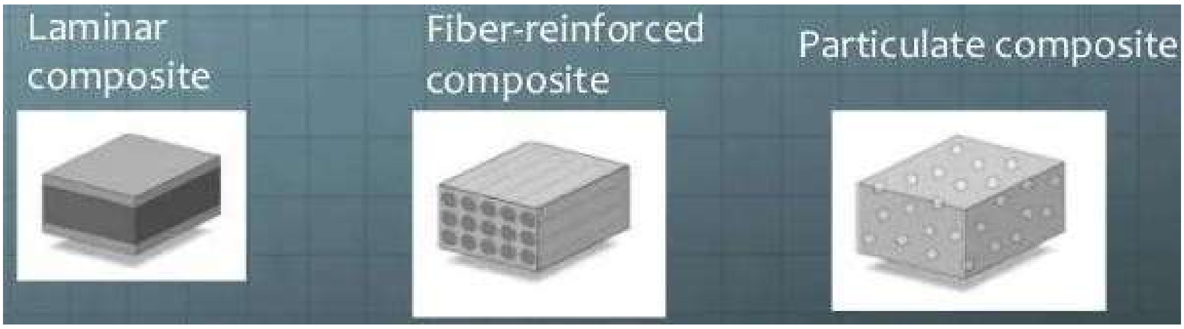


Figure 3 Types of composites

The composites that are studied in this thesis are categorized as particulate composite. The epoxy silica composite which has epoxy as its matrix and silica as the reinforced material or filler material as we will refer to in this thesis.

2.1.2 Epoxy-Silica Composites and their utilities

Epoxy-silica composites are a type of particulate used in various applications, including:

1. AEROSPACE

Epoxy-silica are utilized in producing high-strength and lightweight aircraft components, such as fuselage structures and wing.

2. WIND ENERGY

Epoxy-silica composites are used to manufacture wind turbine blades, which require a combination of strength, stiffness, and durability.

3. SPORTS EQUIPMENT

Epoxy-silica composites are used to make golf clubs, tennis rackets, and other sports equipment that require a combination of strength and flexibility.

4. CONSTRUCTION

Epoxy-silica composites are used in the construction of bridges and buildings, where they provide high strength and durability.

5. MARINE

Epoxy-silica composites are used in the manufacture of boats and ships, where they provide high strength, low weight, and resistance to corrosion.

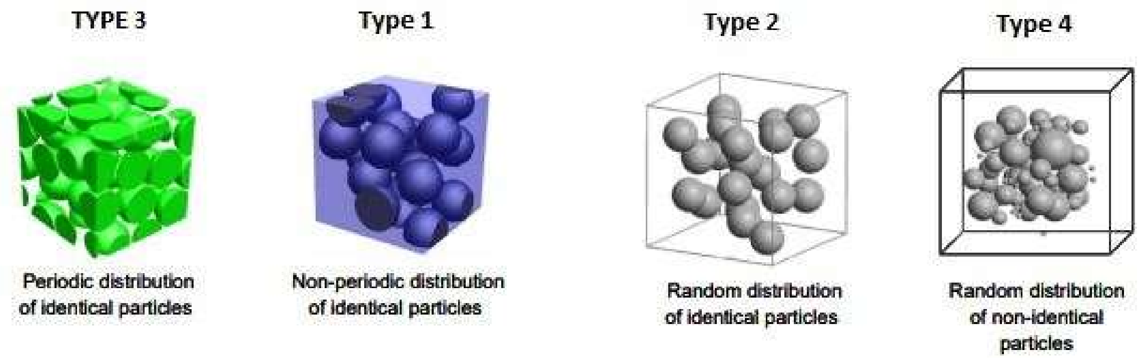
6. ELECTRONICS

Epoxy-silica composites are used in the manufacture of printed circuit boards and other electronic components, where they provide high strength and electrical insulation.

Previous studies have been conducted to study the effect of silica filler and its interface with epoxy [4] and the effect of the size and shape of the silica in the composite [5]. A study of silica based filler on the properties of molding epoxy compounds in terms of viscosity has also been conducted in recent times [6].

2.2 RVE

An RVE is a volume of the material of a size large enough so that any volume of an increased size will be equally representative. [7] Which ensures that test results achieved on an RVE would replicate to test results of full structure. The RVE is generated by the DigiMat [8], a software package that allows the construction of the geometry before it is exported to Abaqus software for meshing the microstructure.



Periodic distribution of identical particles

Non-periodic distribution of identical particles

Random distribution of identical particles

Random distribution of non-identical particles

Figure 4 Types of RVEs generated by Digimat

The provided diagram showcases various categories of sphere-filled RVEs. These RVEs are intended for utilization in multiple research studies, where they will be subjected to diverse parameter variations and boundary conditions. These categories can be classified into distinct groups based on specific characteristics:

- Fully Embedded spheres (no trimming of inclusions on RVE boundaries)
    - Same inclusions size (random distribution in space) - (type 2)
    - Different inclusions size in a given range (random distribution in space) - (type 4)
- Edge Trimmed spheres (allow trimming of inclusions on RVE boundaries)
    - Periodic Geometry on the boundaries - (type 3)

- Same inclusions size (random distribution in space)
    - Non-periodic Geometry on the boundaries - (type 1)
- Same inclusions size (random distribution in space) [9]

The mesh generation for the RVEs is carried out using Abaqus meshing tools. The establishment of boundary conditions and the implementation of numerical homogenization are both achieved through programming in the Python language. [10]

Analysis of boundary conditions indicated that utilizing periodic boundary conditions is suitable for both periodic geometries. Moreover, the impact of particle quantity, relative to particle size, was explored. The findings demonstrated that higher inclusion numbers lead to more consistent homogenized material properties, minimizing statistical variations. The outcomes highlight that a maximum of 40 spherical inclusions is recommended to prevent unfavorable statistical inaccuracies. Consequently, for our study, we selected 30 inclusions as a prudent choice.

Fillers are utilized to enhance the mechanical attributes of polymers, but specific factors significantly impact the overall strength of nano-composites. These factors include matrix-particle interfacial adhesion, particle size, and particle loading. Although the addition of fillers generally leads to improved mechanical properties, outcomes can sometimes deviate from expectations. The study by Dittanet and R.A Pearson [11] explored the influence of different particle sizes on tensile strength. Their findings indicated that nano-sized particles augment tensile strength as their larger surface area enhances matrix-particle interfacial adhesion, enabling effective stress transfer.

Increasing filler content, however, can yield contrasting results due to changes in filler diameter and surface area. This alteration can lead to weakened matrix-particle interfacial adhesion, limiting the nanoparticles' ability to endure external forces. Consequently, the composite's mechanical properties may resemble those of the unmodified resin.

The study by Asif [12] the tensile strength of the 8% filler concentration surpasses that of 9% and 10%. This can be attributed to enhanced interfacial adhesion at lower filler concentrations, where nanoparticles possess greater surface area for improved bonding with the matrix. In contrast, the tensile strength of the 10% filler concentration is lower due to reduced surface area resulting from increased filler content. Weakening interfacial adhesion contributes to diminished mechanical properties hence our study also considers filler concentration at 8%.

2.3 Fatigue and crack propagation

Crack inception and progression are encountered across various engineering disciplines that encompass advanced loading phases of the mechanical response of solids and structures, potentially culminating in failure. [13] Fatigue is the initiation, formation and propagation of cracks in a material due to cyclic loads. The failure occurs due to the cyclic nature of the load which causes microscopic material imperfections to grow into a macroscopic crack. This phenomenon mainly happens but due to multiple load cycles which causes components to lose their strength and get tired, hence it is called fatigue. [14] Qualitatively there are three stages of fatigue:

2.3.1 Crack initiation

This stage encompasses the inception of cracks and the initial growth of small cracks. It marks the initial phase where cracks emerge within minuscule material microstructures or in regions with a notable concentration of voids. In these minute sites, the cracks give rise to continuous slip bands that extend along the plane experiencing the greatest shear stress (positioned at a 45-degree angle from the applied load direction) under cyclic loads, where stress alternates. These sites elude visible detection and give rise to exceptionally focused areas of heightened stress.

2.3.2 Crack propagation

During this phase, when cracks attain a critical size, minor cracks extend across 2-3 grain boundaries, which are considerably larger than the material's microstructure. The heightened stress concentration in these regions leads to plastic stresses at the tips of the cracks. These recurring plastic stresses gradually align perpendicular to the maximum principal stress, causing the micro-crack to progressively propagate over an indistinct region of fatigue fracture.

2.3.3 Fracture

During this phase, if the crack that originated in the second stage keeps growing due to available energy, it will persist until it reaches a point of tensile failure.

For instance, if a test specimen undergoes the stages of crack nucleation and growth, and the crack's propagation persists, it progressively diminishes the cross-sectional area of the specimen. Eventually, this weakening effect culminates in a situation where the component becomes so compromised that only one additional load application is sufficient to trigger final and complete fracture. The specific type of fracture - whether ductile, brittle, or a combination thereof- depends on various factors such as the type of metal, the stress levels involved, the surrounding environment, and more. [15]

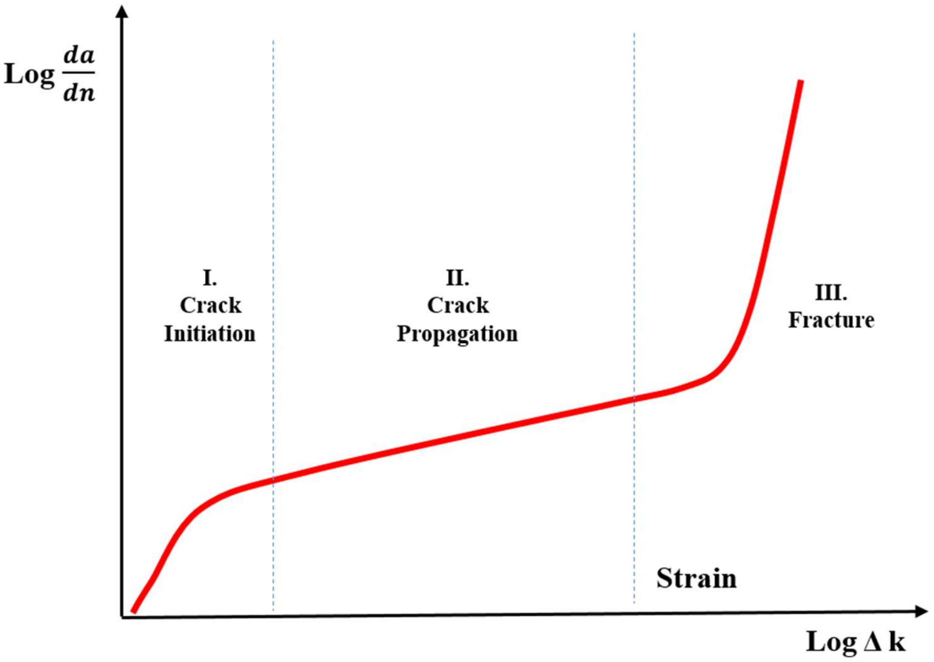


Figure 5 Graph for stages of fatigue failure

The eXtended Finite Element Method (XFEM) is a technique rooted in the partition of unity concept. It is especially well-suited for simulating crack propagation phenomena, even when the crack path is not known beforehand. Numerically, it is commonly realized through dedicated standalone codes. Although efforts have been made to integrate XFEM into commercial Finite Element Analysis (FEA) software, its adoption remains limited. Among such software, Abaqus stands out as the most notable, incorporating XFEM capabilities. Nevertheless, due to its relatively recent introduction, the effectiveness of XFEM in Abaqus has been demonstrated primarily in basic benchmark problems involving linear elastic material models, where trustworthy results have been established.

CHAPTER 3: RVE GENERATION

3.1 Digimat

The first step to conduct our study was to generate representative volume element (RVE) in digimat software. Digimat comes in handy when dealing with composites specially. E-Xstream engineering is the creator and vendor behind the software suite called Digimat, an advanced technology for modeling materials across multiple scales. This innovation significantly expedites the development of composite materials and structures. At the core of the 10xICME Solution, Digimat is instrumental in conducting intricate analyses of materials at the microscopic level. It also produces micromechanical material models that are well-suited for bridging the gap between micro and macro scales. These Digimat material models facilitate the integration of processing simulation and structural finite element analysis (FEA). This advancement enables a transition towards more predictive simulations by encompassing the influence of processing conditions on the ultimate performance of the manufactured component. [16]

To generate material geometry, we used FE module of digimat. The module required to feed in the material properties such as Young's modulus and poisson ratio.

Properties of epoxy are defined as:

Young's modulus = 3.35 GPa

Poisson Ratio as 0.3

Properties of silica are defined as:

Young’s modulus 74.8 GPa

Poisson Ratio as 0.19

Silica is used as spherical inclusions in the polymeric epoxy matrix. The shape of RVE is kept as cuboidal with the geometry as 100mm by 100mm by 100mm.

The constant factor amongst all the generated RVEs was kept as the number of inclusions to be 30. We varied volume fraction by 1%, 5%, 10%, 15% and 20%. We also generated RVE with 30% volume fraction of the filler material. The point to be noted over here is that when we are altering the volume fraction, the shape and size of the inclusion is being varied to fill in the space in the matrix.

3.1.1 Generated RVEs with different filler concentration

The following diagrams displays the composites with different filler concentration. The spheres in the diagram are representing silica particles. Wireframe view is provided for a better understanding.

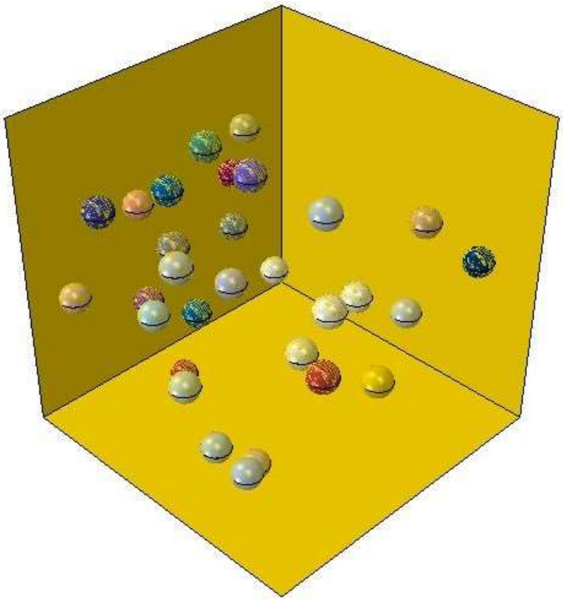


Figure 6 Epoxy-silica composite with 1% volume fraction of silica

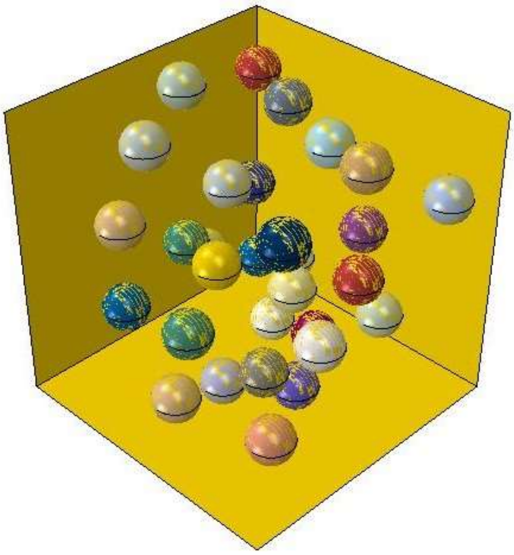


Figure 7 Epoxy-silica composite with 5% volume fraction of silica

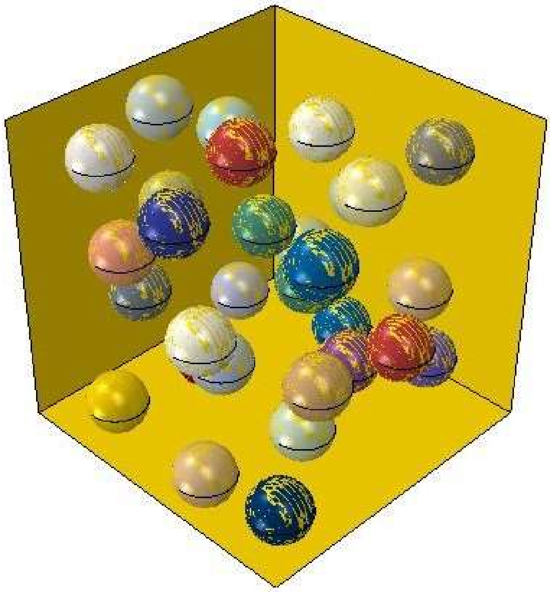


Figure 8 Epoxy-silica composite with 10% volume fraction of silica

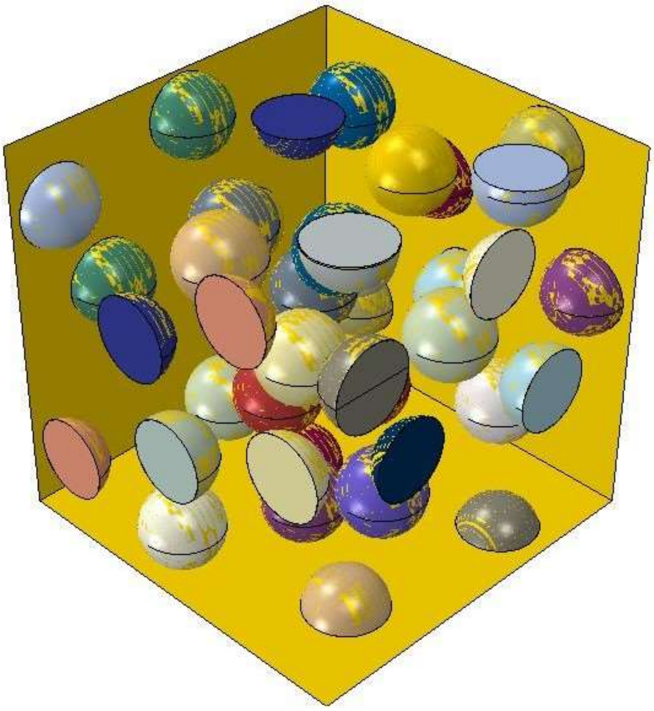


Figure 9 Epoxy-silica composite with 15% volume fraction of silica

Figure 10 Epoxy-silica composite with 20% volume fraction of silica

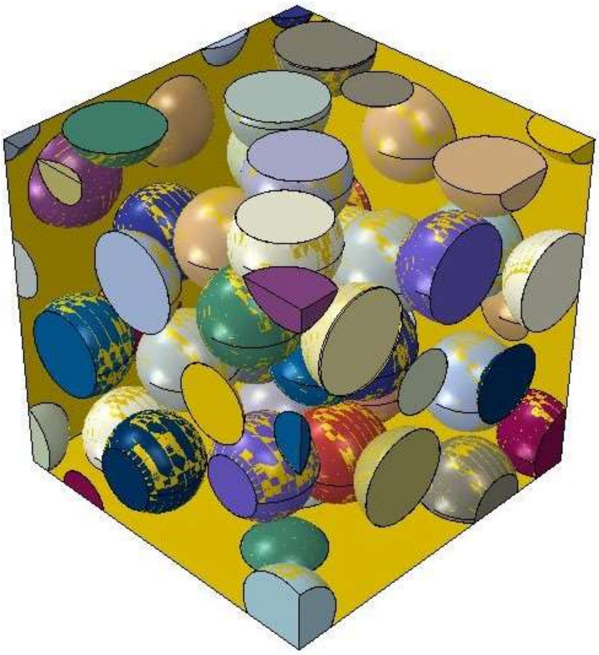


Figure 11 Epoxy-silica composite with 30% volume fraction of silica

3.2 Abaqus

Though Digimat is capable of running finite element analysis but due to the objective of performing crack propagation analysis, Abaqus was used. These composites were exported in the form of script to Abaqus for further analysis. Abaqus and Digimat both are unit less softwares and both run on python script. This facilitates the exportation of geometry constructed on Digimat to Abqaus.

Abaqus is a product of DS Simulia. It can deal with complex systems, any kind of geometry and it can also simulate reinforced concrete, glass ceramics, polymers, composites etc.

CHAPTER 4: FINITE ELEMENT ANALYSIS OF RVE

The finite element analysis is basically a numerical technique which is used to predict and simulate material behavior in different scenarios. It is mostly used to inspect vulnerabilities in designs in structures and prototypes. [17] Importing a geometry into Abaqus from Digimat made the analysis a bit easier as the geometry was predefined.

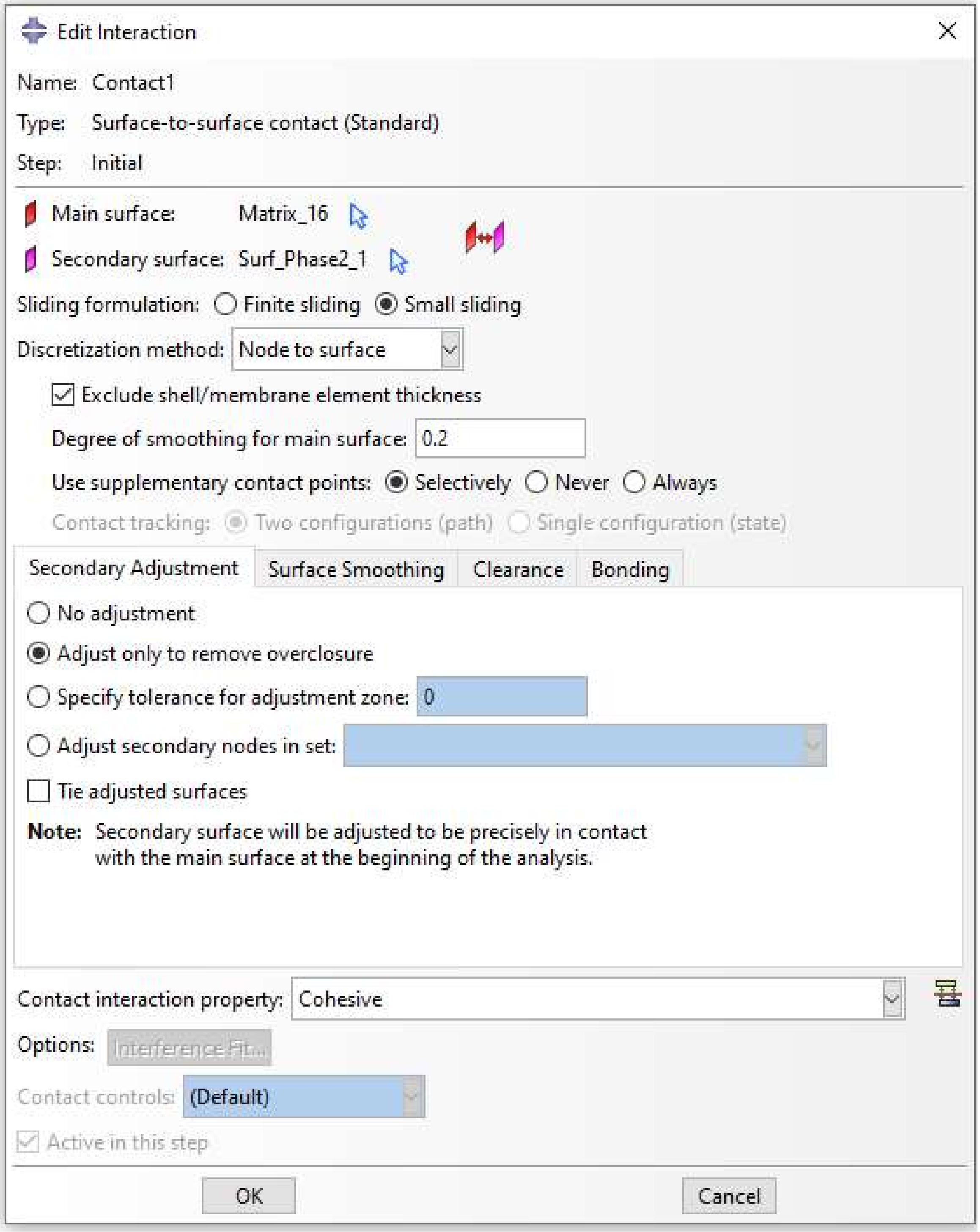
To begin with, details that were used for dealing with volume fraction of 30% are stated in the text below.

4.1 Meshing

The total number of nodes are 50981 and total number of elements in the geometry of 30% volume fraction are 74487. 53891 are linear tetrahedral elements of type C3D4 and 20596 quadratic tetrahedral elements of type C3D10M.

4.2 Contact Formulation and damage criterion

Micro-modelling technique is utilized to simulate the matrix and inclusions. Contact interactions is one of the key features that should be defined for accurate results. These contacts are between the inclusions and the matrix. We utilized surface based contact as compared to general contact due to cohesive behavior. Surface based cohesive behavior provides a simplified way to model cohesive connections with negligibly small interface thicknesses using the traction-separation constitutive model. For slide formulation, small sliding is selected. Node to surface discretization method is used and smoothening is performed. Overclosures are removed to avoid convergence issue. A picture of selected options in Abaqus is given below.



Name: Contact1

Type: Surface-to-surface contact (Standard)

Step: Initial

Main surface: Matrix_16

Secondary surface: Surf_Phase2_1

Sliding formulation: ○ Finite sliding ● Small sliding

Discretization method: Node to surface

☑ Exclude shell/membrane element thickness

Degree of smoothing for main surface: 0.2

Use supplementary contact points: ● Selectively ○ Never ○ Always

Contact tracking: ● Two configurations (path) ○ Single configuration (state)

○ No adjustment

● Adjust only to remove overclosure

○ Specify tolerance for adjustment zone: 0

○ Adjust secondary nodes in set:

☐ Tie adjusted surfaces

Note: Secondary surface will be adjusted to be precisely in contact
with the main surface at the beginning of the analysis.

Contact interaction property: Cohesive

Options: Interference Fit...

Contact controls: (Default)

☑ Active in this step

Figure 12 Contact formulation

Cohesive properties are used to simulate between the inclusions and matrix. The parameters required for developing cohesive behavior are:

- Linear elastic traction separation
- Damage initiation criteria
- Damage evolution law

Elastic response of the interacting surfaces depends upon linear traction separation relationship till the initiation of damage. Generally this relationship is defined by normal (K_{nn}), tangential (K_{tt}) and shear (Kss) stiffness coefficients values which are given in the table below. These properties are defined as:

Cohesive Behavior		
K_{nn}	**K_{ss}**	**K_{tt}**
1E+11	1E+11	1E+11

Table 1 Cohesive behavior properties

For crack analysis, we needed to define damage criterion which was selected as quadratic traction and fracture energy is chosen to be 220 J.

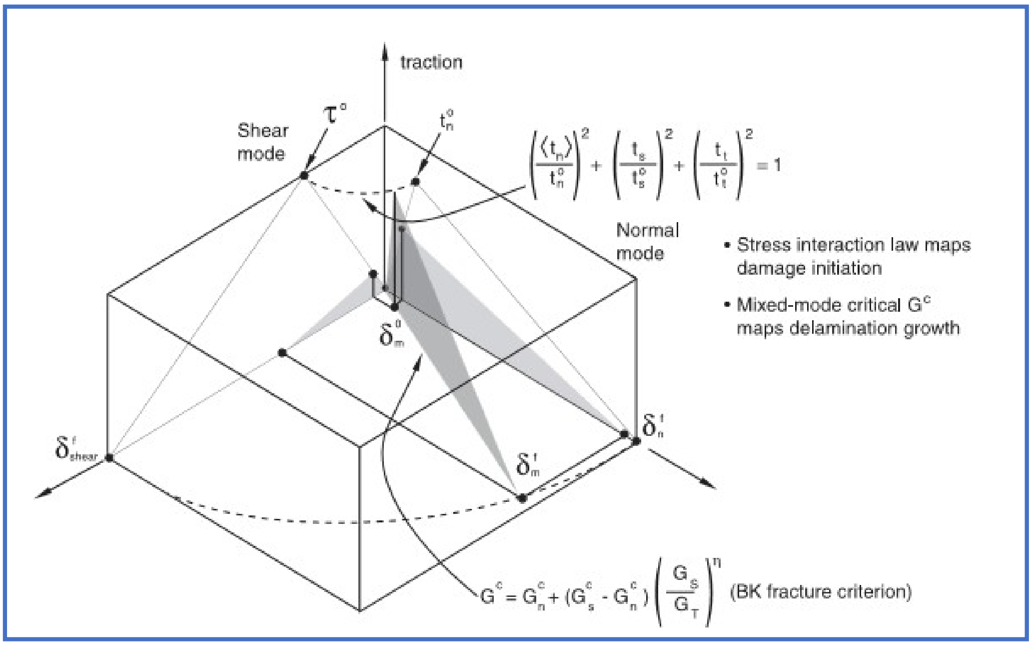


Figure 13 Traction-separation curve (3D)

For the generation of stress-strain graphs, boundary conditions are set as follows:

The boundary conditions were defined in Abaqus as lower and upper Surfaces are constrained by Multi-Point constraints with Respective Reference Points. Upper Reference point is set to have a displacement of 5mm. We have fixed lower Reference point for all Degree of freedom

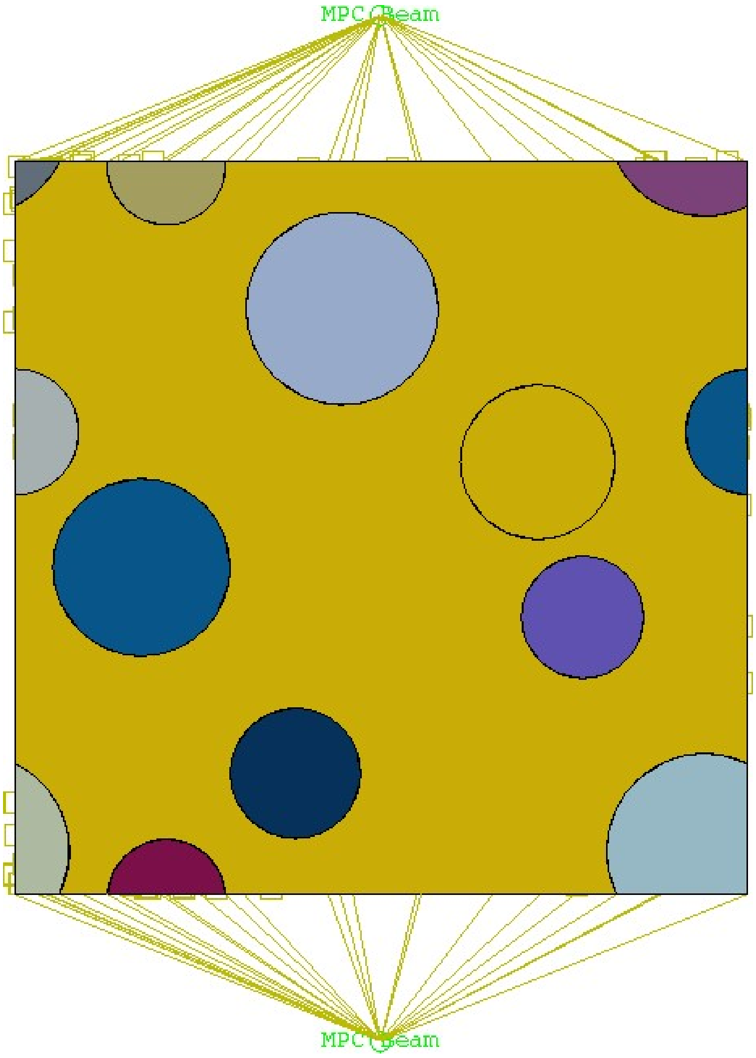


Figure 14 Set boundary conditions

4.3 Crack Propagation

The study of crack propagation cannot be carried out in the normal module of Abaqus. For crack analysis, extended finite element module is used. Due to simulation challenges, 2D composite with 1% inclusion randomly distributed is generated using Digimat software and imported to Abaqus.

Initial crack is located in the 2D plane as crack initiation is a step before crack propagation. Force is applied on the geometry which leads to the propagation of the crack throughout geometry.

The final outcome of the study is discussed comprehensively in the next chapter.

CHAPTER 5: RESULTS AND CONCLUSIONS

5.1 Finite Element Analysis Results

The generated results are compiled and discussed in this chapter.

The order that is followed is graphical results are provided generated by Abaqus and then the findings are tabulated.

Later in this chapter, crack propagation analysis is also discussed.

5.1.1 Graphically generated FEA results of different filler concentration composites

- ***1% filler concentration***

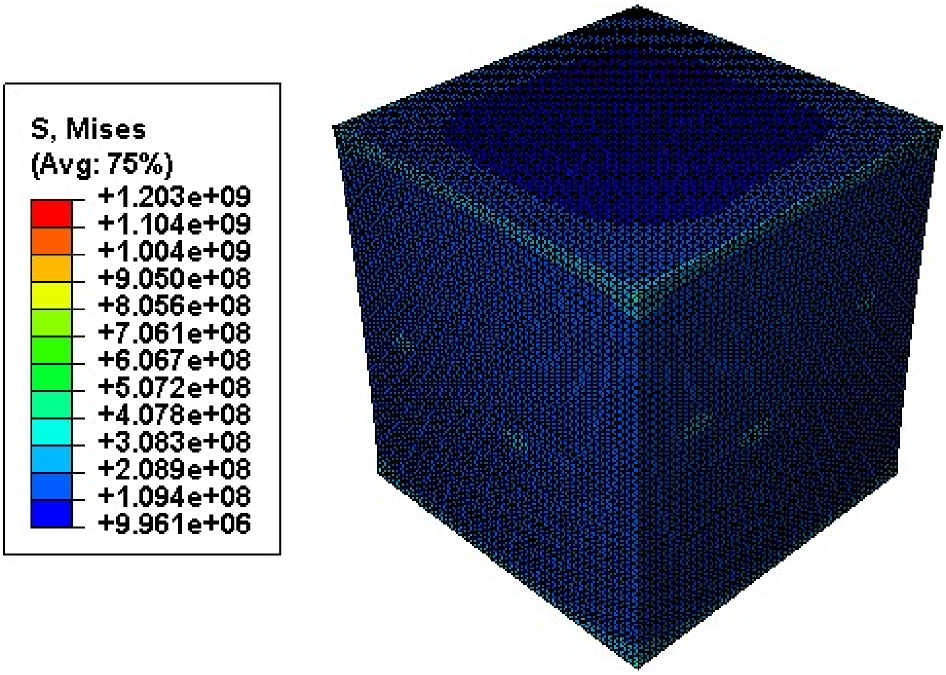


Figure 15 FEA of 1% concentration

- ***5% filler concentration***

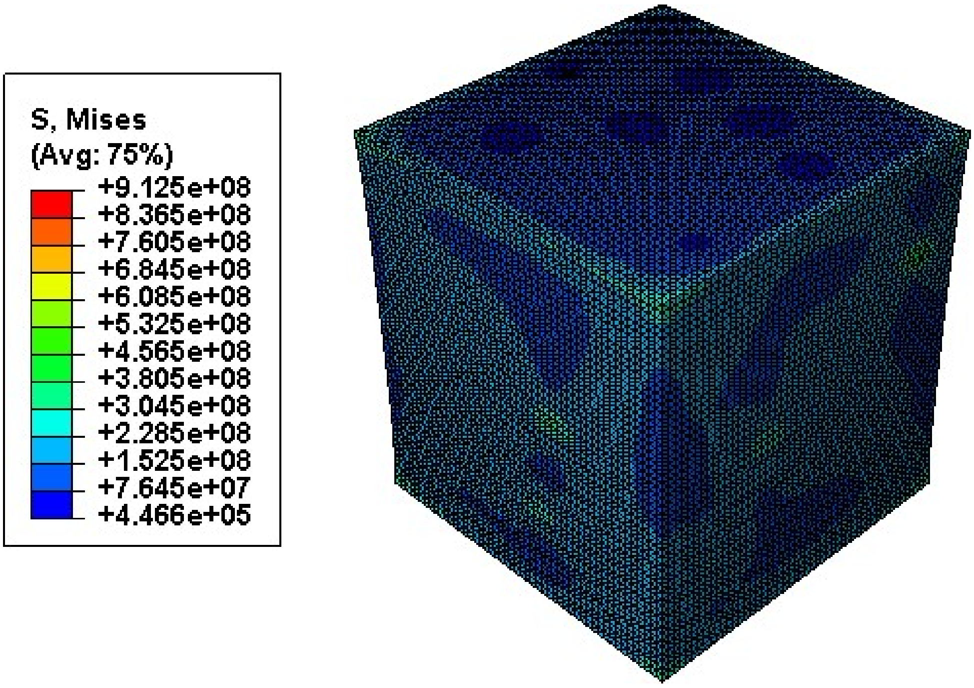


Figure 16 FEA of 5% concentration

- ***10% filler concentration***

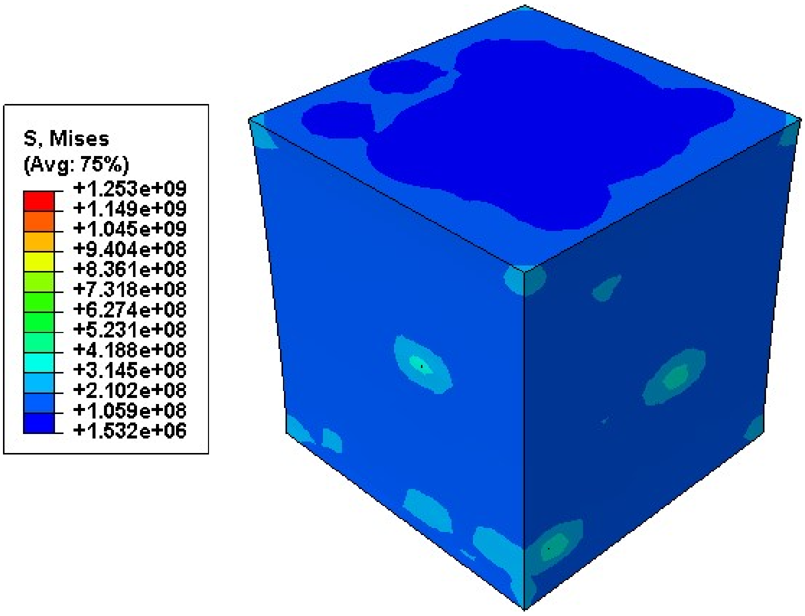


Figure 17 FEA of 10% concentration

- ***15% inclusions***

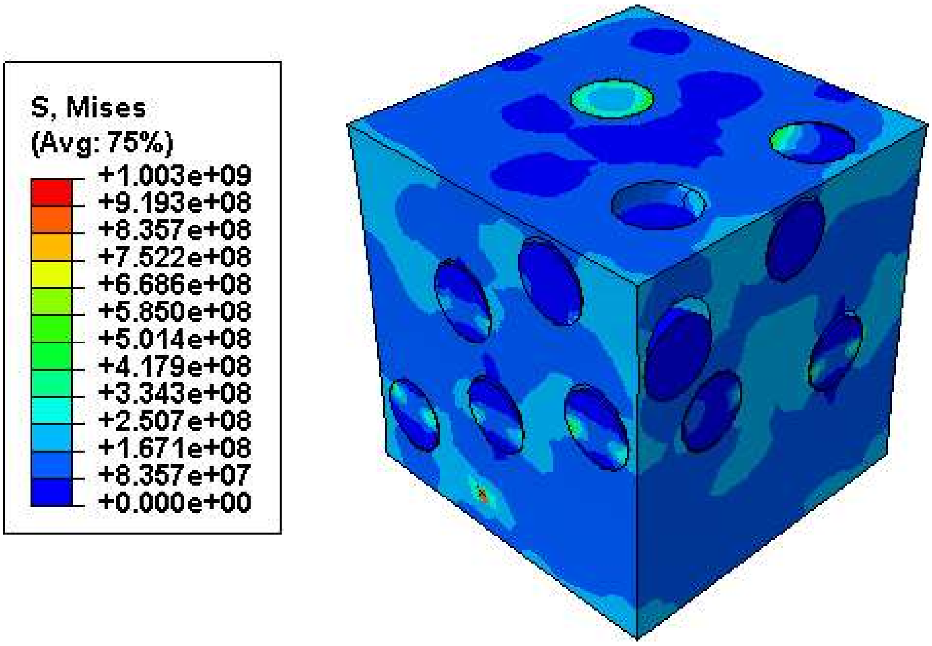


Figure 18 FEA of 15% concentration

- ***20% inclusions***

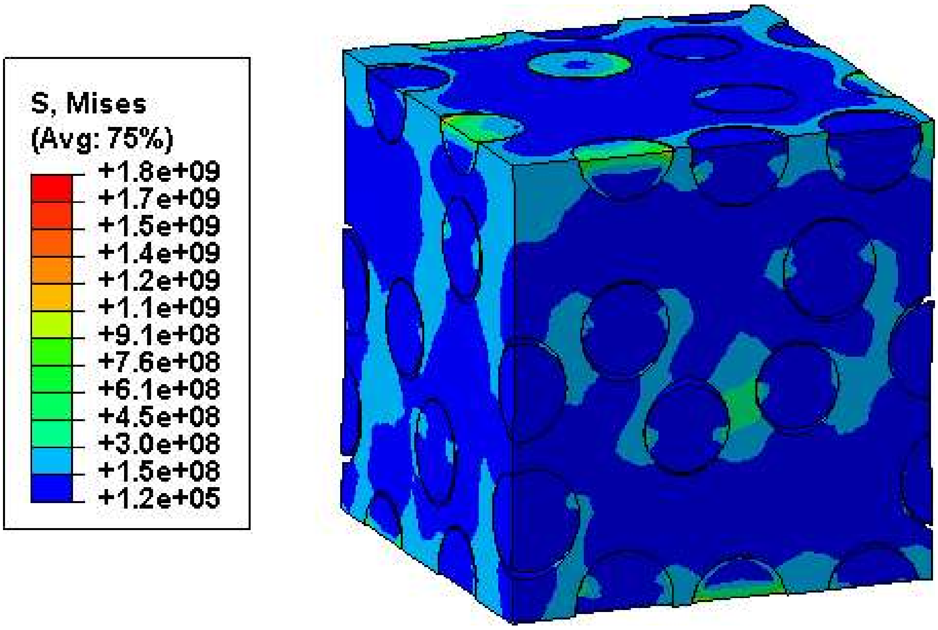


Figure 19 FEA of 20% filler concentration

- ***30% inclusions***

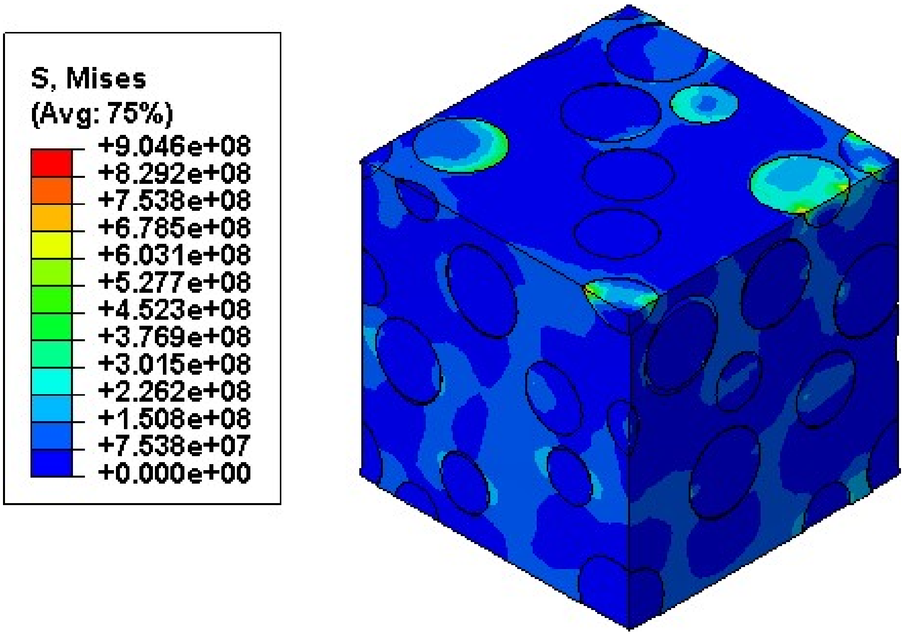


Figure 20 FEA of 30% concentration

Table 2 tensile strength as per FEA of different filler concentration

Filler concentration	**Tensile strength (Pa)**
1%	1.20E+09
5%	9.13E+08
10%	1.25E+09
15%	1.00E+09
20%	1.80E+09
30%	9.05E+08

As we can read through the graphical representation, the composite with 20% filler concentration shows the maximum stress before failure in the same conditions. To create a numerical correlation, the software tool of Archanoid [18] was used. The generated data through Abaqus was fed into the software. A polynomial equation of degree 5 is produced. This equation provides an insight of the stress the composite can bear before failure.

Equation:

$$\textit{Tensile strength} = 1805457039 - 79160900141x + 2060657862859x^2 - 20785634385786x^3 + 88490347414254x4 - 130934600943875x^5$$

where x denotes percentage of filler concentration in the epoxy-silica composite

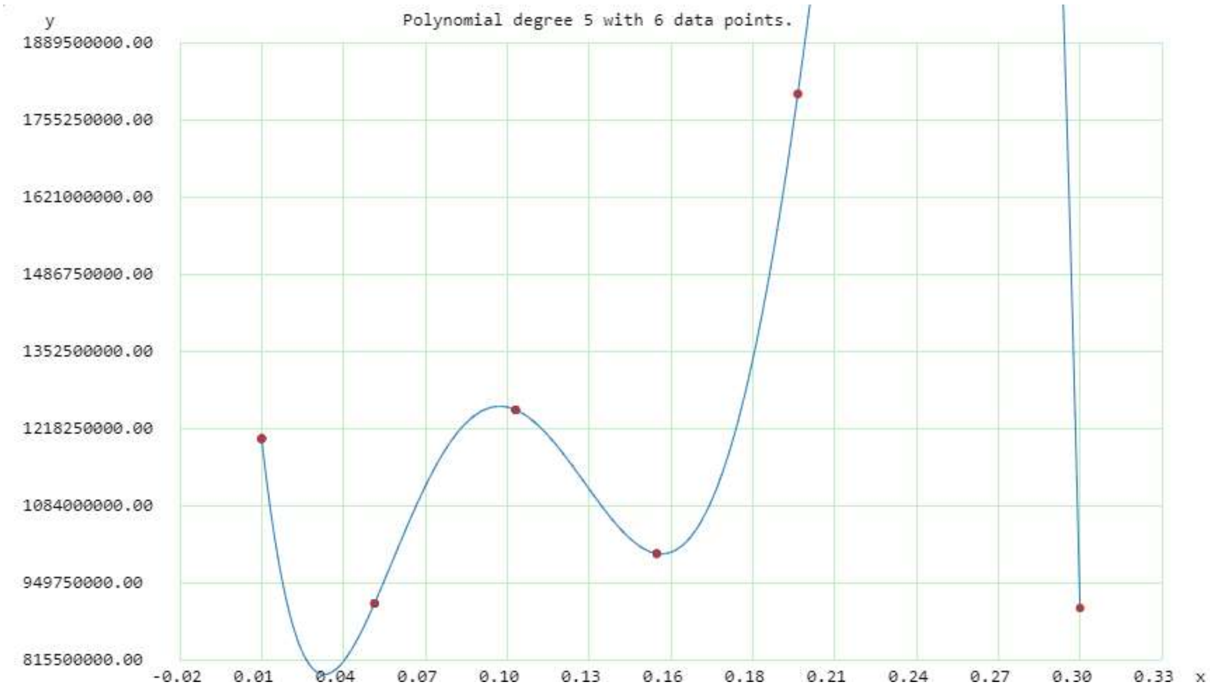


Figure 21 Generated graph of the obtained equation

Solving the equation for optimum filler concentration results in below values:

Filler concentration	Tensile strength
20%	1.80E+09
21%	2.18E+09
22%	2.62E+09
23%	3.07E+09
24%	3.49E+09
25%	3.83E+09
26%	4.01E+09
27%	3.93E+09
28%	3.48E+09
29%	2.52E+09
30%	9.05E+08

Table 3 Tensile strength at different percentages of filler material

Above results suggest that 26% filler concentration results in the highest tensile strength hence being the optimum selection in an epoxy-silica composite.

5.1.2 Stress-strain graph of different filler concentration composites

Comparative stress-strain graph of RVEs with different filler concentrations with two conditions are generated below:

5.1.2.1 Comparative graph with perfectly bonded conditions

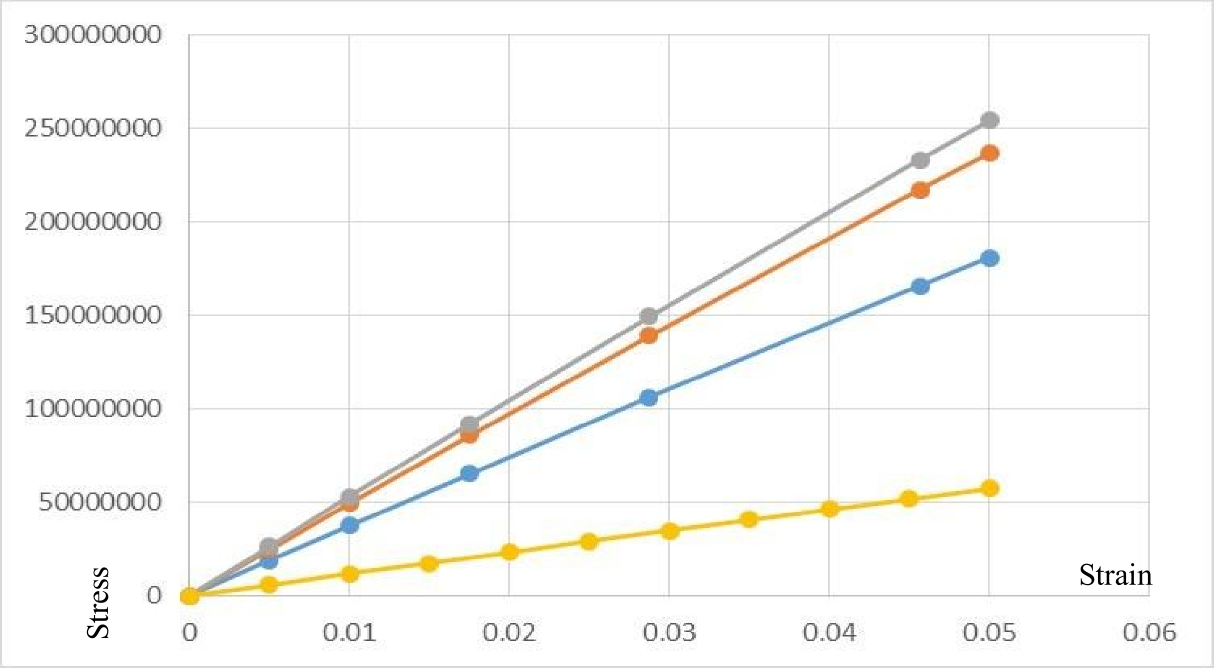


Figure 22 Stress against Strain graph of composites with different filler concentrations perfectly bonded conditions

This graph shows that in perfectly bonded conditions, the stress to strain ratio increases. In other words, it is difficult to deform the composite with higher filler concentration as compare to the one with less filler concentration.

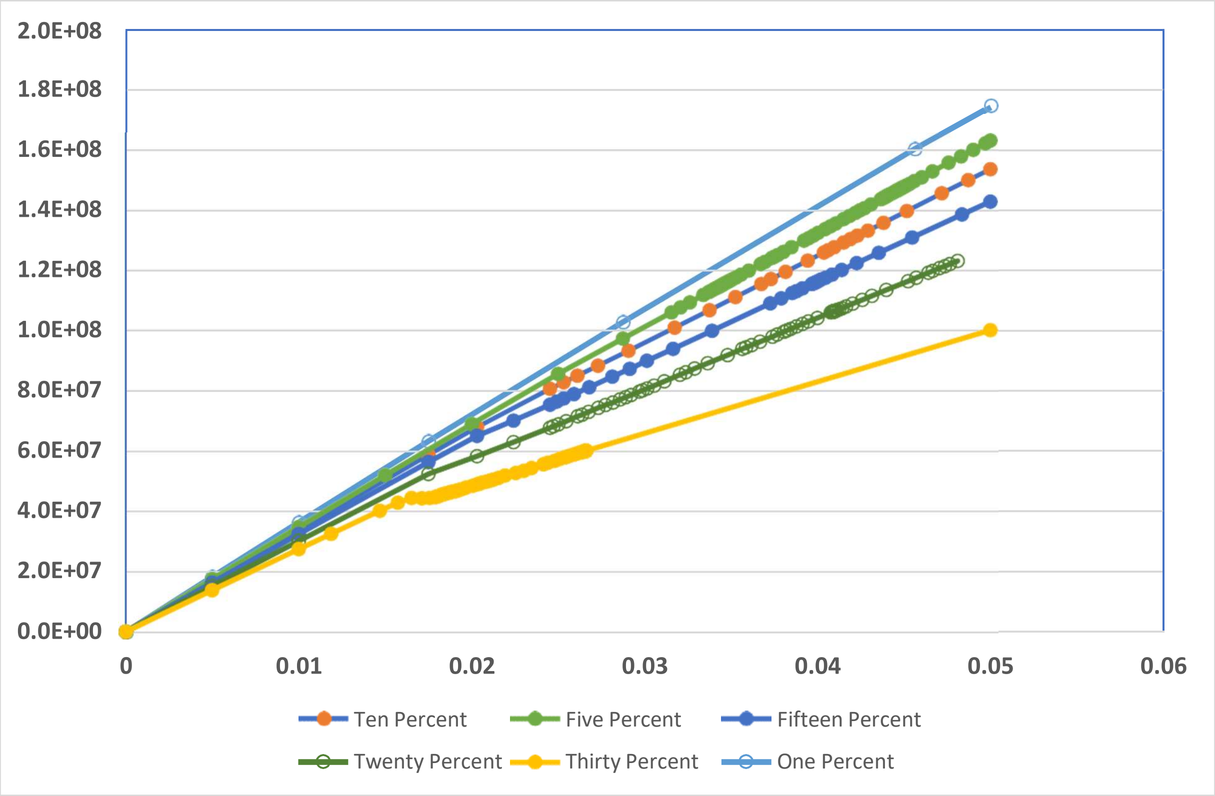


Figure 23 Stress against Strain graph of composites with different filler concentrations with debonding

The generation of graph and FEA by Abaqus enabled us to establish a relationship between tensile stress and filler concentration.

5.2 Crack Propagation Results

After the initial crack in the composite with filler concentration of about 1%, provided the fracture energy was set to be 220 J, the crack propagates quite linearly until the point, it comes in contact with the first inclusion. The crack is observed to induce stress amongst the inclusions present in the geometry which then initiates further cracks within the geometry. It is to be noted the maximum stress region is still the one where crack is progressing.

Due to time constraint, the study could not be completed for other filler concentrations which may be a motivation for other researchers to research on. The propagation of crack as per Abaqus XFEM module is graphically illustrated below for a better understanding.

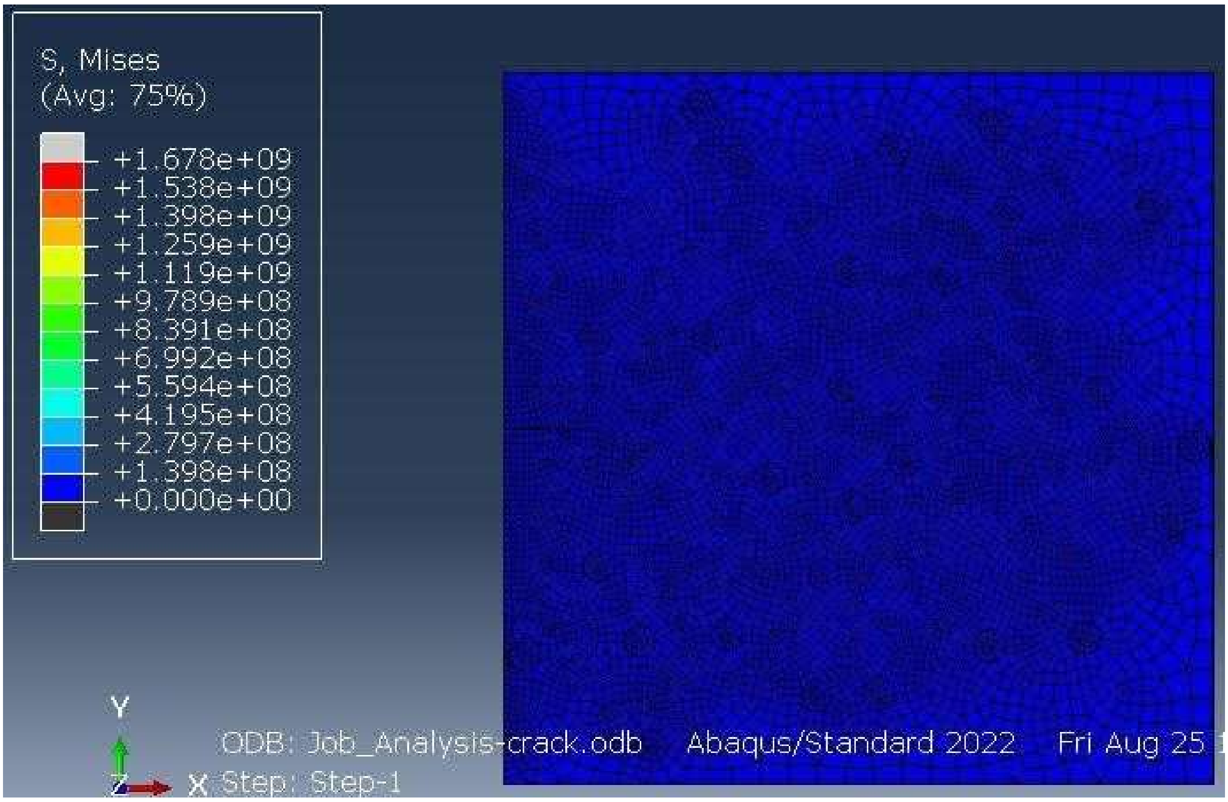


Figure 24 Crack initiation

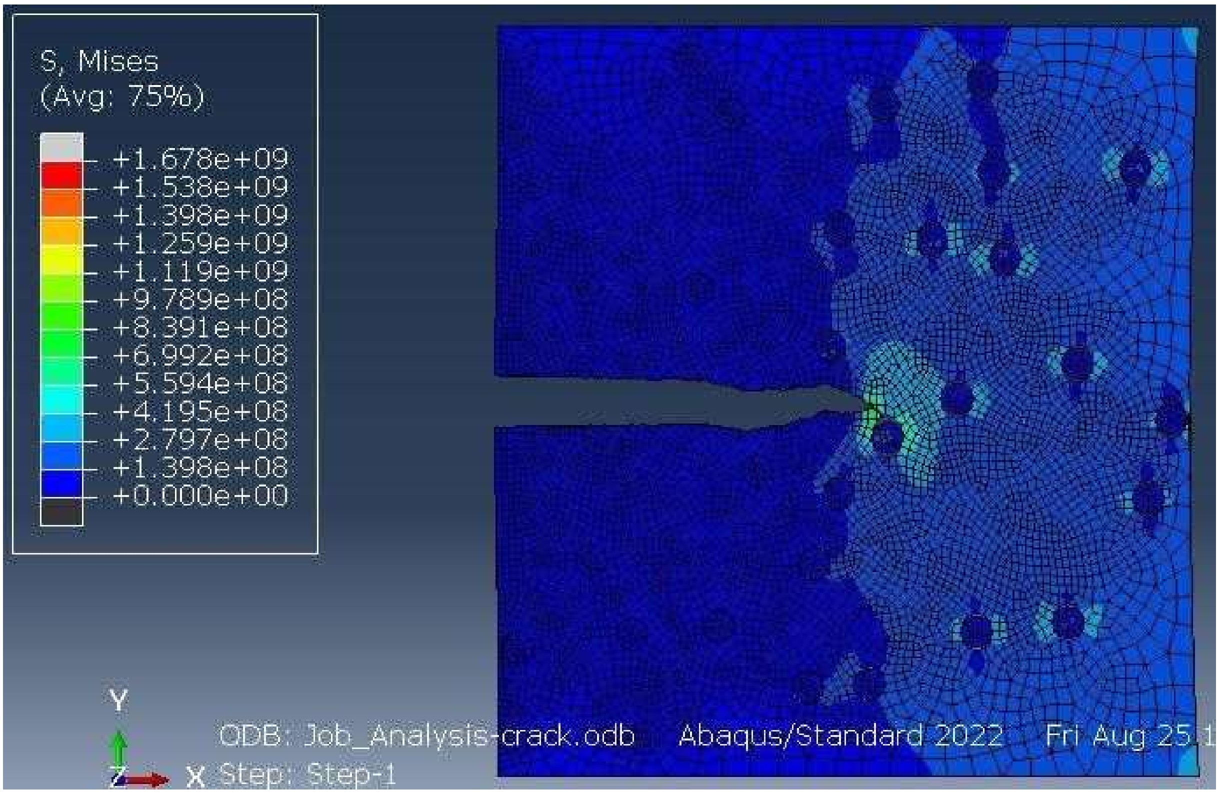


Figure 25 Crack when it hits inclusion

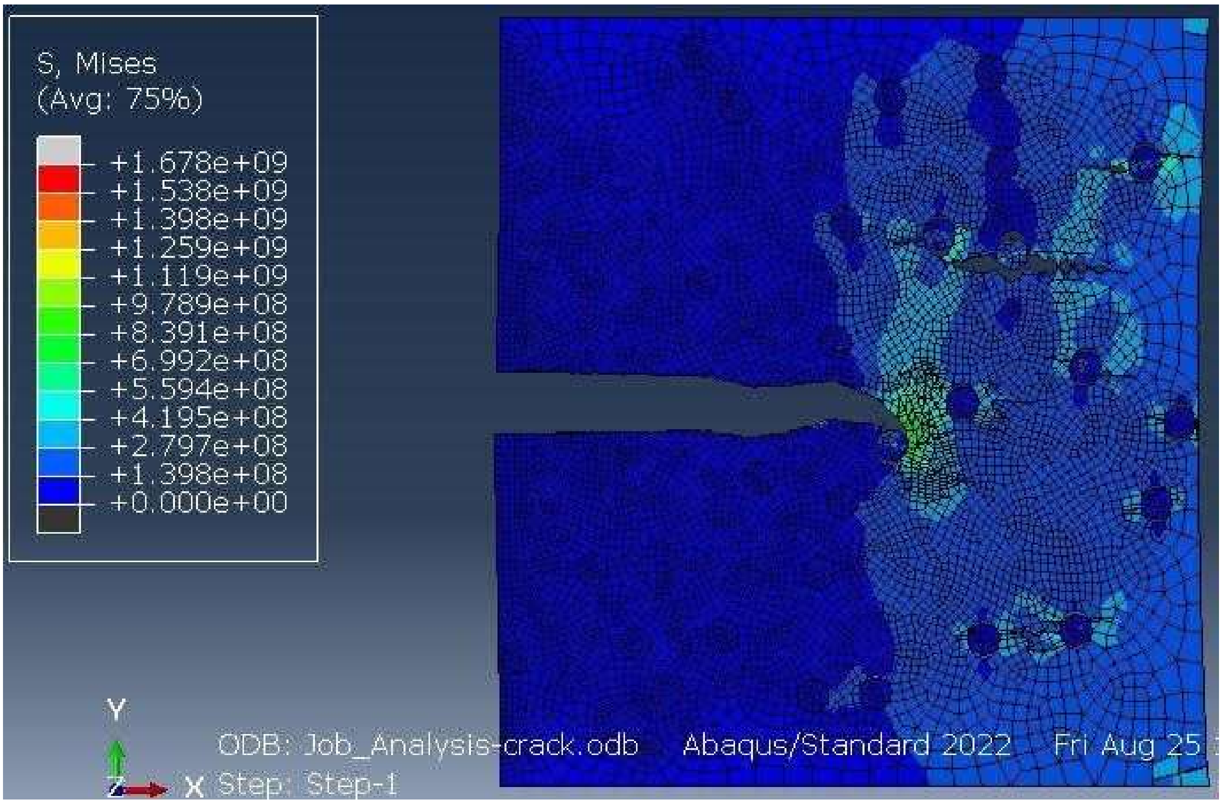


Figure 26 Cracks are generated within the geometry

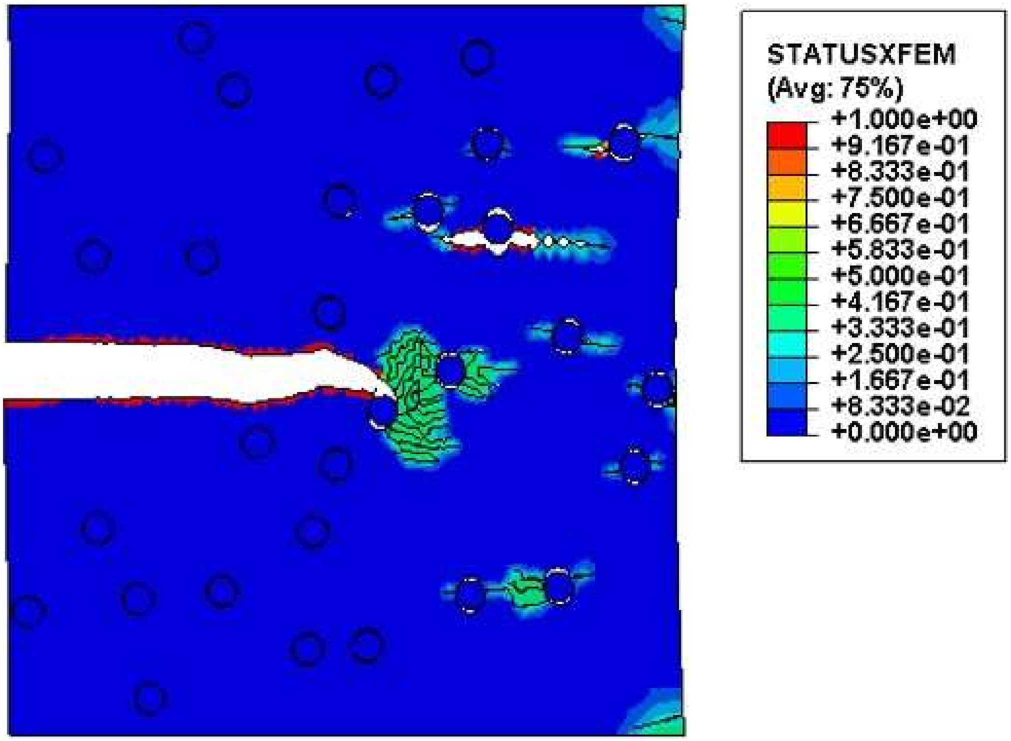


Figure 27 Stress distribution in crack propagation

5.3 Conclusions

- With a steady rise in the filler concentration within the composite material, an obvious trend is observed:

i. With perfectly bonded conditions the stress to strain ratio increases with increase in filler concentration. Representing that with higher filler concentrations, deformation is difficult.

ii. The stress to strain ratio has a decreasing gradient. This occurrence is crucial as it suggests deformation will occur at higher percentages with a lesser force.

- The sophisticated stress distribution profiles, precisely generated through Finite Element Analysis (FEA) simulations through Abaqus made the findings interesting. Notably, when evaluating composites characterized by varying filler concentrations of silica, a visible pattern occurs: the composite composition with a 26% filler concentration seems to have a distinctive advantage. Specifically, it demonstrates the most favorable scenario concerning the justification of maximum stress under analogous loading conditions.

- Under crack propagation analysis, observation of the influence of inclusions on the trajectory of crack development is noticeable. The presence of these inclusions hinders propagating cracks behavior, resulting in an alternative pathway of crack progression. This suggests with increase in filler concentration, the crack pathways will be deviated more due to the probability of encountering inclusions more.
- The crack propagation is observed to have a ripple effect on other inclusions once it hits the first inclusion on its way. This phenomenon suggests the complexity of the occurrence of damage and its dependence on structural constituents in predicting generic mechanical response.

The amalgamation of these insights, gathered from both empirical observation and computational simulations, emphasizes the complex nature of composite materials under mechanical inspection. Through this analysis, one can explore the true potential for engineering materials with enhanced mechanical characteristics. This convergence of material science, numerical analysis, and insightful interpretation highlights the continuing journey towards the discovery of underlying principles that govern the mechanical behavior of composite materials.

CHAPTER 6: FUTURE SCOPE

The study can be extended further and utilized for future works. This study addresses FEA of different filler concentrations in composites keeping the number of inclusions constant. It is also accompanied with the crack propagation analysis of composite with 1% filler concentration. However, more can be done in this regard. Following are points that present future scope of this study:

- Study can be performed with different number of inclusions, thereby extracting the effect of different number of inclusions on the properties of composite material.
- Crack propagation at different concentrations of filler material can also be performed in 3D, which was one of the limitations that came across due to time constraint.
- Proper numerical model can be formulated then for different filler concentration.
- Different geometry other than cubic can also be studied and results can be compared to present study. In this case, the effect of geometry on the properties of composites can be studied comprehensively.
- As per the findings of this thesis, we can set up an experimental setup to validate the findings.

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