Multiscale Computational Analysis of Mechanical Properties in Graphite Nano-Composites Using ANSYS for Enhanced Structural Performance

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Abstract: This paper investigates the advancements in engineering materials and the application of the Finite Element Method (FEM) in structural analysis. It focuses on the significant material science developments during World War II, emphasizing the creation of superalloys, composites, and nanomaterials, and their pivotal roles in the aerospace and nuclear sectors. The study explores the adaptability and challenges of FEM in analyzing complex structures, utilizing ANSYS software for evaluating two different material specimens: one without nanofillers and another infused with silicon dioxide nanofillers. The research underscores the importance of accurate modeling and analysis in engineering design and the critical role of FEM in predicting composite material behaviors under varied conditions, while also reflecting on the historical evolution of these materials and methodologies and their impact on contemporary engineering and technology.

Keywords: Composite Materials, FEM, Ansys, Graphite, Nanofiller

1. INTRODUCTION

Throughout history, the brilliance of human innovation has frequently been showcased through significant breakthroughs in materials and technology, crucial for surmounting the challenges of their times. The era of World War II marked a particularly intense phase of material innovation, propelling metallurgists and engineers to achieve unprecedented levels of discovery. The outcomes of their endeavors have profoundly influenced a wide array of industries, especially aerospace and nuclear sectors. This period was pivotal in the evolution of engineering materials, seeing remarkable advancements in the creation of high-performance materials including superalloys, composites, and nanomaterials, which have become integral in modern engineering, especially in aerospace and nuclear applications.

Superalloys, consisting mainly of nickel, iron-nickel, and cobalt, have played a critical role in jet engine applications, prized for their superior heat resistance and consistent mechanical performance even at elevated temperatures [1]. Their durability under harsh conditions has made them invaluable in aerospace and nuclear contexts, with nuclear power plants, for instance, utilizing nickel-based superalloys in key components like reactor cores and control rods [2]. Composites, on the other hand, represent a diverse group of multi-phase materials, merging high strength, lightweight, and corrosion resistance, qualities that have propelled them to prominence in the construction of aircraft, space vehicles, automobiles, and various other sectors.

Nanomaterials, at the forefront of contemporary material science, offer innovative solutions to longstanding challenges. Carbon Nanotube Metal Matrix Composites (CNT-MMCs) are particularly notable for their exceptional tensile strength and electrical conductivity, attracting considerable research interest for aerospace applications [3]. The field of nanotechnology is spearheading a transformative shift in material science, with nanomaterials increasingly replacing traditional metals in aerospace and other advanced industries due to their enhanced mechanical and environmental properties [4]. Today's engineering landscape boasts over 50,000 different materials, providing engineers with an expansive range of choices to fulfill the complex requirements of current projects.

Structural analysis, a key component of research, relies heavily on tools like the Finite Element Method (FEM), with software such as ANSYS, NASTRAN, and POINTWISE playing a crucial role in assessing the mechanical behavior of material structures and aiding in the design and optimization of engineering systems. This ongoing development and application of new materials and technologies highlight the dynamic synergy between human creativity and the demands of the era. The transition from wartime innovations to contemporary engineering achievements narrates a story of relentless human effort and unwavering innovative spirit.

In summary, the diverse array of engineering materials, born from historical necessities and creative human thought, continues to drive innovation across numerous industries. The pivotal contributions of metallurgists and engineers in pushing the boundaries of material science and technology stand as a lasting tribute to human ingenuity and the endless possibilities of engineering in shaping our future.

2. GRAPHITE NANOFILLERS

Metamorphic rocks found across continents like South America, Asia, and North America are rich sources of graphite, a form of carbon that naturally occurs in these regions. The formation of graphite involves intense heat and pressure, leading to the emergence of sedimentary carbon compounds that typically manifest as either flakes or layers within these rocks [5]. There are three primary variants of natural graphite – flake graphite, crystalline vein graphite, and amorphous graphite – each differing in physical properties due to their unique formation processes [6].

Extensive research over the past century has unveiled graphite's extraordinary natural properties. It is known for its exceptional stiffness, inherent resistance to chemical reactions, and the ability to maintain its strength at temperatures exceeding 3600°C [6], [7]. Graphite's anisotropic nature, which results in higher electrical and thermal conductivity along its layers compared to its poorer conductivity across them, makes it particularly suitable for lubrication purposes due to the ease with which its carbon layers can slide over each other [8]. Beyond lubrication, graphite's versatility extends to applications in water purification, advancements in optical fiber technology, and the development of fuel cells [9].

The specific heat capacity of a material, fundamentally linked to its atomic structure, is defined as the thermal energy required to increase the temperature of one gram of the substance by one degree Celsius [10]. Tavman et al. [11] used differential scanning calorimetry (DSC) to measure the heat capacity of graphite nanocomposites within a temperature range of 40-100°C, finding that graphite's specific heat not only increases with temperature but also exceeds previously reported figures. Pulse current heating is another method for measuring graphite's specific heat, involving the brief application of heat to a small graphite sample and monitoring the temperature change. In their research, Matsumoto and Ano [12] applied this method to ribbon-shaped graphite at temperatures ranging from 1500 to 3000 K, establishing a direct relationship between specific heat and temperature increases.

The experimental findings regarding graphite's specific heat generally align with the theoretical calculations of the Debye model, which estimates the phonon contribution to a solid's heat capacity [13]. Some variances at extremely low temperatures have been noted, potentially due to impurities or defects in the graphite. Recent studies have also explored the specific heat of graphene, a single layer of graphite, noting its distinct electronic and thermal properties that set it apart from bulk graphite [14].

3. FINITE ELEMENT METHOD

In the realm of engineering and design, particularly when navigating the complexities of aircraft assemblies, marine structures, and intricate mechanical parts, finding precise solutions can be challenging. Engineers have access to a range of approximate methods to tackle these challenges, including the Galerkin's method, Finite Difference Method, Finite Volume Method, and notably, the Finite Element Method (FEM) [15]. FEM distinguishes itself as an exceptionally adaptable tool for analyzing structures with intricate geometries, diverse material types, and various boundary conditions and load scenarios [16].

Finite Element Analysis (FEA) is segmented into three crucial phases: Modeling (also known as the Pre-Processing phase), Analysis and Solution, and finally, the Post-Processing stage for evaluating results [17]. In the initial phase, the problem is defined by its dimensions (1D, 2D, or 3D) and involves selecting appropriate material models, elements, meshing techniques, and applying the correct structural or thermal boundary conditions. The type of load applied, whether thermal, mechanical, electrical, or magnetic, is tailored to the specific requirements of the application [18].

Modern engineering leverages various software tools to streamline these processes. Solid Works, for example, is widely used for its precision in modeling, ensuring adherence to exact dimensions and constraints [19]. Once a model is created, its compatibility across different platforms is vital. Saving models in IGS format ensures they can be seamlessly transferred to analysis platforms like ANSYS, a powerful tool for the analysis phase. ANSYS allows for additional layers to be added, especially for composite materials, and prepares the model with the necessary loads and boundary conditions [20].

The final phase, post-processing, is critical for engineers and designers as it reveals how structures respond under different load conditions, whether static, dynamic, or influenced by thermal changes, impact, fatigue, or torque. This analysis phase often precedes product development, offering detailed insights through tables, graphical representations, structural deformations, and even animations [21]. A key feature of software like ANSYS is its ability to generate detailed stress distribution diagrams, which are invaluable for comparing experimental data, theoretical models, and stress values derived from FEA, thus ensuring the creation of robust and dependable designs [22].

4. SPECIMEN MATERIALS, TYPES AND METHODOLOGY

In this study, three distinct material specimens are utilized. The initial specimen serves as a control, lacking any nanofiller within its matrix. The second is integrated with silicon dioxide nanofillers, and the third incorporates graphite nanofillers into its matrix. The models employed in this experiment, pre-designed using various CAD software, align with ASTM standards for different mechanical tests conducted in the software. For example, the tensile strength model complies with ASTM D 638M, while models for compression, impact, flexural, and hardness tests adhere to ASTM D 1621, ASTM D 256 (Izod/Charpy), ASTM D 790, and ASTM E18-22 (Rockwell's/Brinnel's), respectively [23].

The research leverages ANSYS software to pinpoint potential failure points in tensile, compression, and bending test simulations. By dividing the test specimen into multiple discrete elements, the software emulates the real-time stress impacts on each element, cumulatively providing an overall stress assessment of the specimen [23]. The probe feature in the software is utilized to determine the maximum stress or force experienced by each element.

This study encompasses various numerical iteration software solutions, refined over time, for both linear and non-linear analysis of complex meshed structures. Typically, a uniform finite difference mesh is applied to the specimen, with boundaries delineated and approximated using a mix of horizontal and vertical lines. Basic shapes like triangles and rectangles are used for real-time stress analysis on 2D test samples within finite element modeling software. While finite element models are not inherently superior to finite difference models, they are customized for specific scenarios based on their context and usability. However, finite element modeling software is notably adept at handling complex, varied geometric shapes.

Finite element discretization in this study involves transforming a test problem (generally a continuous sample specimen) into finite, discrete elements. This method involves representing the undefined field variable through assumed approximation functions within each element, commonly referred to as interpolation functions in numerical and computational analysis.

The construction of structures using composite materials poses unique challenges, particularly due to the simultaneous design requirements for the material and the structure. The analysis encompasses the examination of structures made from composite materials at both the micro and macro levels. ANSYS Mechanical APDL, a renowned finite element analysis (FEA) tool, is used for its user-friendly graphical interface and comprehensive help system. Each user action within the GUI generates ANSYS command lines, recorded in a .log file, making the software's functionality transparent to the user.

Ansys offers a range of structural analysis software tools, enabling engineers of diverse expertise to tackle complex structural engineering challenges more efficiently. By employing this suite of tools, engineers can perform finite element analyses (FEA), customize and automate solutions for structural mechanics, and explore various design scenarios. Utilizing this software early in the design process aids in cost reduction, streamlines design cycles, and accelerates product market entry.

The analysis process within the software follows specific steps:

1. Initiate ACP (pre) and input materials like epoxy-saturated E-glass.
2. Determine the required number of layers and their respective thicknesses.
3. Create a static structure and integrate the specified material.
4. Test the material within the static framework, adjusting the applied force to identify the point of failure.
5. Gradually adjust a parameter until the force threshold leading to material failure is identified.

Analysis results suggest that the specimen is likely to fail under conditions of compression, 3pt bending, and tensile stress at approximately 200 KN, 20 KN, and 20 KN, respectively. Considering an expected 1KN to 10KN improvement in the secondary specimen, ANSYS data indicates the second specimen's superior performance during mechanical testing. Thermal testing also shows promising results, though the increase in thermal capacity is not as significant as that in mechanical tests. This research employs a Finite Element Analysis approach for Strengthened Composite, methodically layering fiber and resin with an alignment ranging from 0 to 90 degrees. Underlying assumptions include treating the composite as a homogenous material, approximating resin thickness at 0.00015mm, disregarding imperfections for flawless composite perception, ensuring perfect fiber alignment, and uniform fiber distribution. The composite is fixed along the x-axis, and a detailed meshing process is conducted, resulting in a three-dimensional Finite Element mesh for accurate simulation outcomes.

5. MECHANICAL TESTING OF THE SPECIMENS USING COMPUTATIONAL (APPROXIMATION) ANALYSIS.

5.1. TENSILE TEST

The examination was conducted to highlight the relationship between the stress and strain exerted on the substance, aiming to delineate its novel material characteristics. Subjected to a load of 78KN, the material, measuring 2032x1.905x1 cm, underwent testing. The following outcomes were observed for the control Composite.

	Normal Stresses	Maximum Principal stresses	Strain Energy
Minimum	-354.92 MPa	-1.978e-13 MPa	9.3636 e-003 MJ
Maximum	5013.6 MPa	5512.6 MPa	3.0295 MJ
Average	82.963 MPa	279.19 MPa	-
Total	-	-	-

For graphite nanofiller, following data was recorded:

	Normal Stresses	Maximum Principal stresses	Strain Energy
Minimum	-451.63 MPa	-4.3006e-13 MPa	9.3636 e-003 MJ
Maximum	4544.8 MPa	4999.1 MPa	3.0295 MJ

Average	56.3993 MPa	248.32 MPa	-
Total	-	-	-

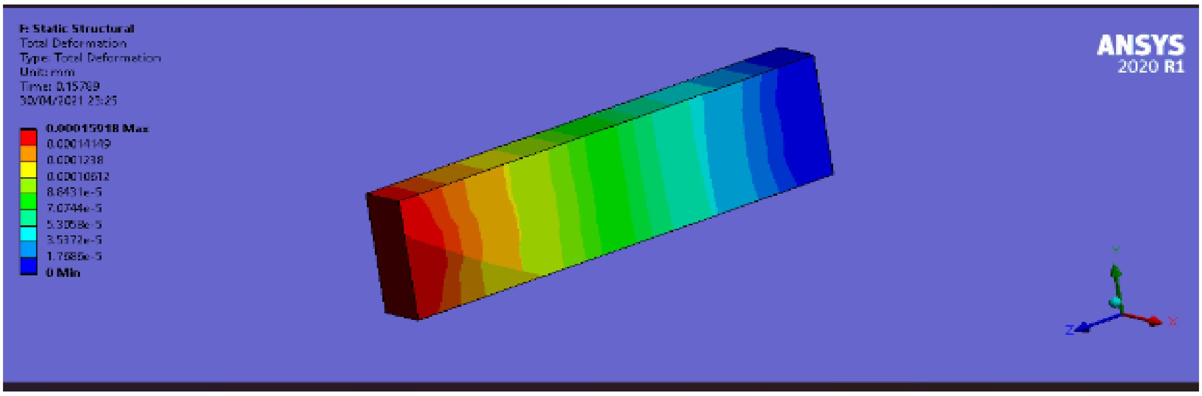

Fig-1 Tension Control Specimen Normal Stress

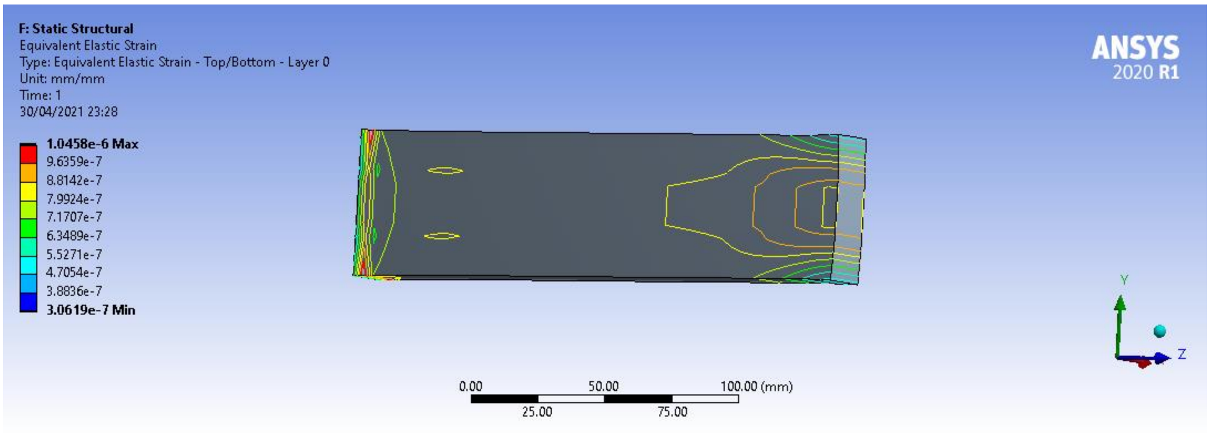

Fig-2 Tension Graphite Specimen Normal Stress

5.2. COMPRESSION TEST

Compression tests were conducted to determine the peak compressive strength of high silica fiberglass upon the addition of nanofillers. The sample was crafted in compliance with ASTM standards and was evaluated using a universal testing apparatus. A compressive force of 78KN was first applied to the control sample and subsequently to the Graphite sample. In Ansys, the specimen's dimensions were configured to 30mmx30mmx30mm. A force was exerted at the central point of the specimen, while the base remained stationary. The results of the simulated tensile strength are presented below.

S.NO	Sample	ULTIMATE Tensile Load	Ultimate Tensile Strength
1	Control Sample	78KN	10.618 MPa
2	Graphite Sample	78KN	18.9305MPa

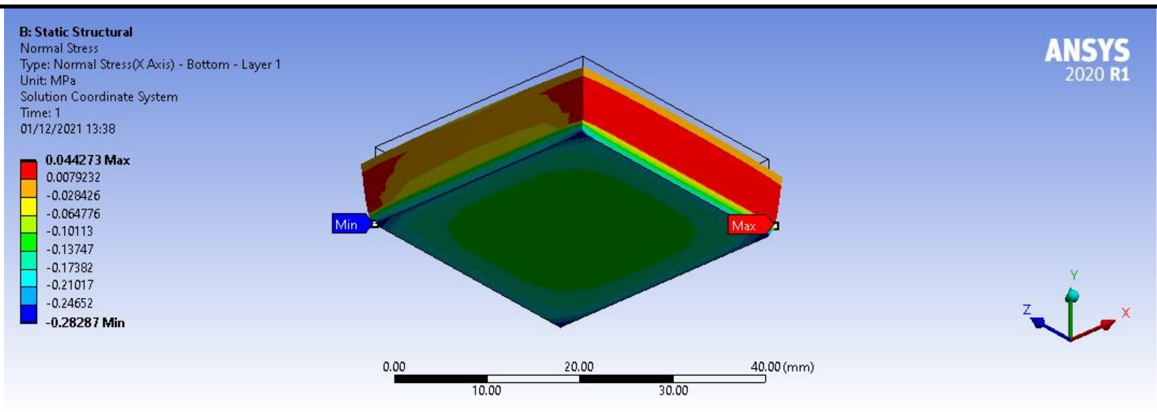

Fig-3 Control Composite Normal Stress Analysis (Compression)

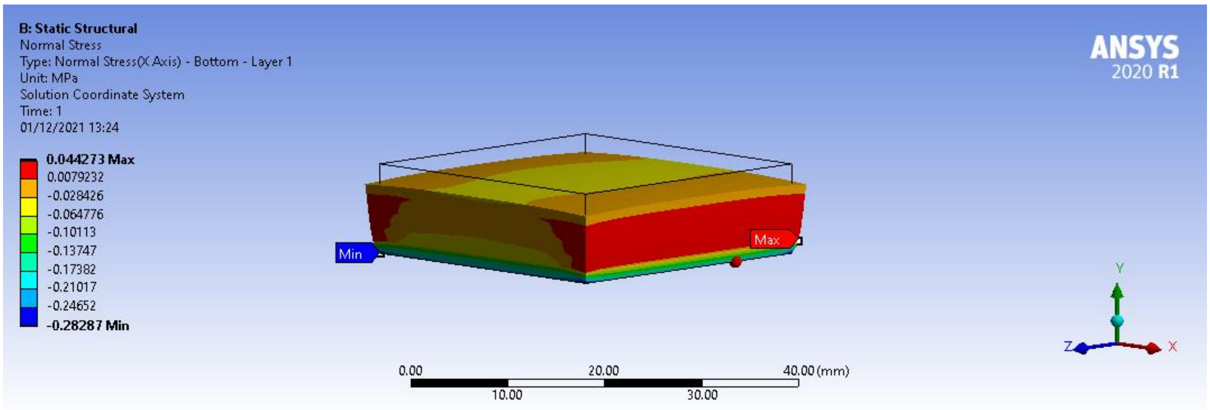

Fig-4 Graphite Specimen Normal Stress Analysis (Compression)

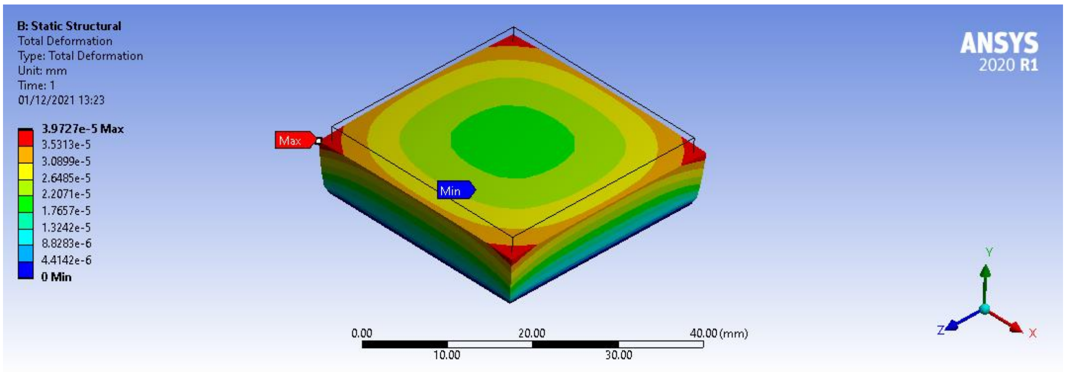

Fig-5 Control Specimen Total Deformation Analysis (Compression)

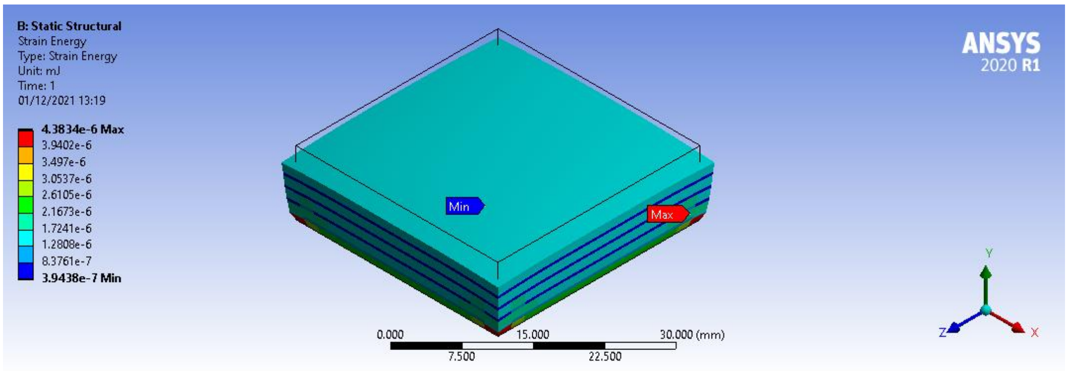

Fig-6 Graphite Anysis Total deformation (Compression)

5.3. THREE POINT FLEXURAL TEST

The assessment was carried out to identify the diverse stress types resulting in the maximum deformation of the specimen and to evaluate the material's resilience and flexibility. An initial load of 78KN was exerted on the control sample followed by the graphite sample, and the outcomes were juxtaposed. The dimensions of the specimen were configured as 400mmx30mmx30mm, with a 26KN force applied at three distinct points on the sample, while its base remained stationary. Following the simulation, the observed stress and deformation metrics are detailed below.

S.NO	Type of specimen	Type of stresses	Stress Rate	Deformation Rate
1	Control Composite	Normal Stress	326.5MPa	0.98216mm
		Elastic Strain	0.86794mm	
2	Graphite Composite	Normal Stress	319.29MPa	0.67657mm
		Elastic Strain	0.42072mm/mm	

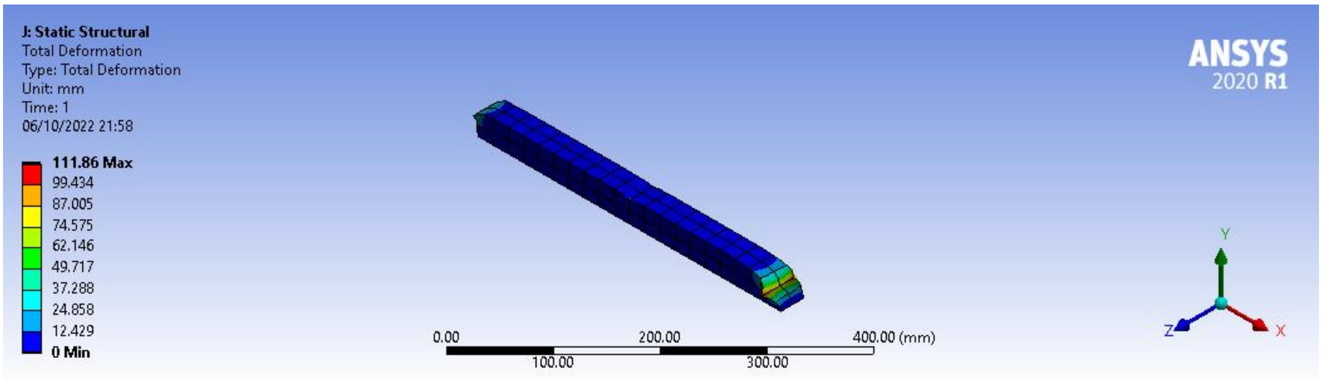

Fig-7 3-Point Bending Control Specimen Total Deformation

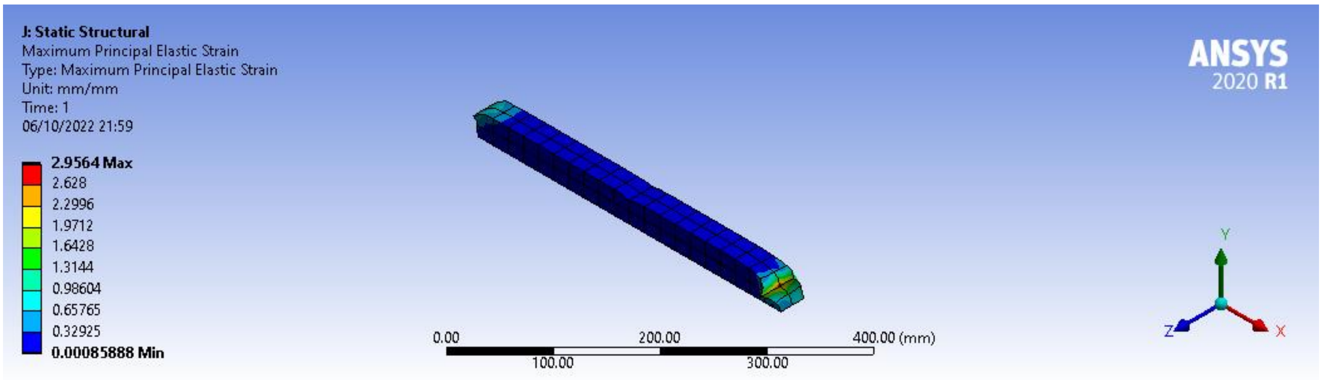

Fig-8 3-Point Bending Control Specimen stress Formation

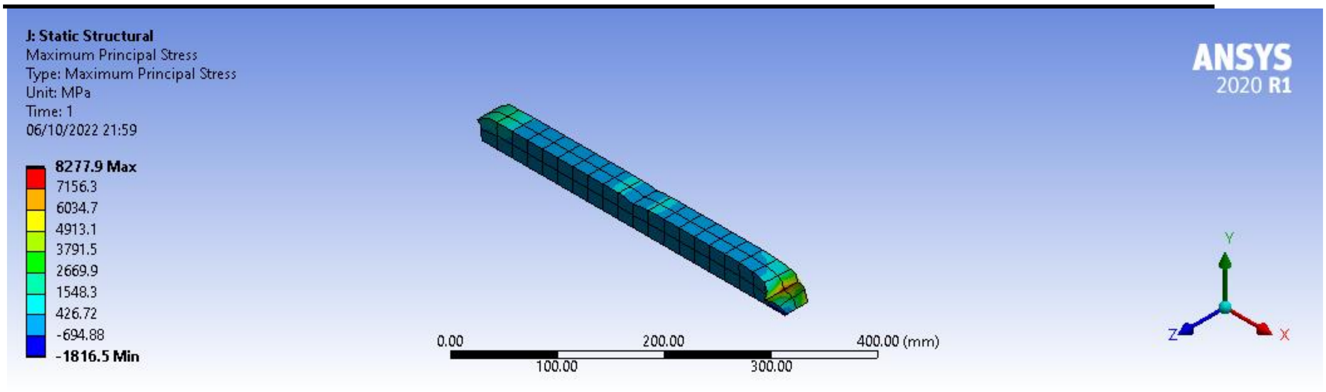

Fig-9 3-Point Bending Control Specimen Strain Analysis

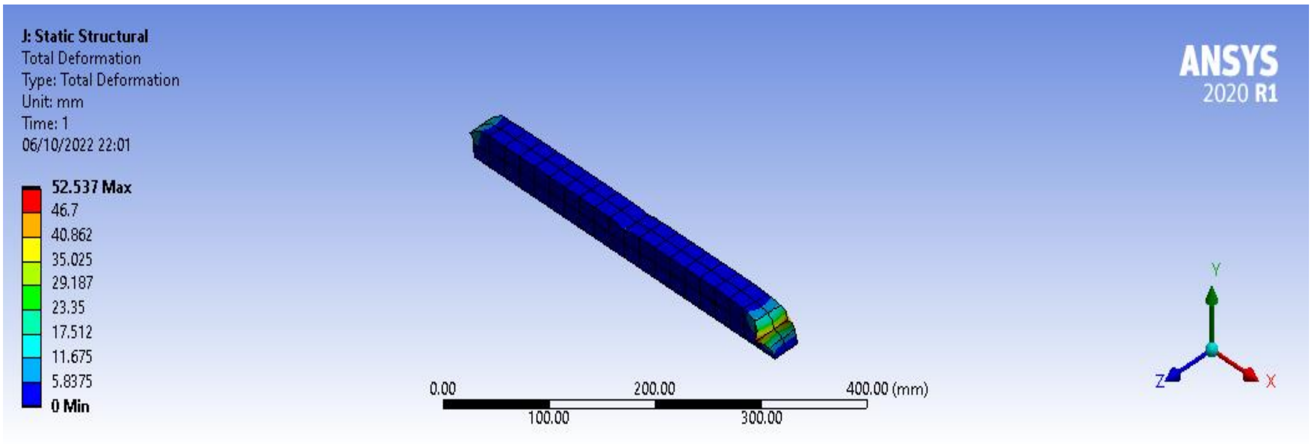

Fig-10 3-Point Bending Graphite Specimen Total Deformation

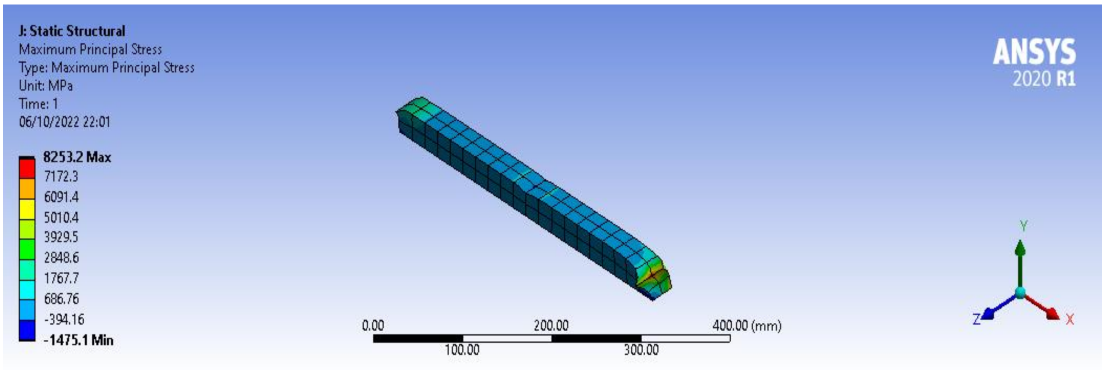

Fig-11 3-Point Bending Graphite Specimen Strain Analysis

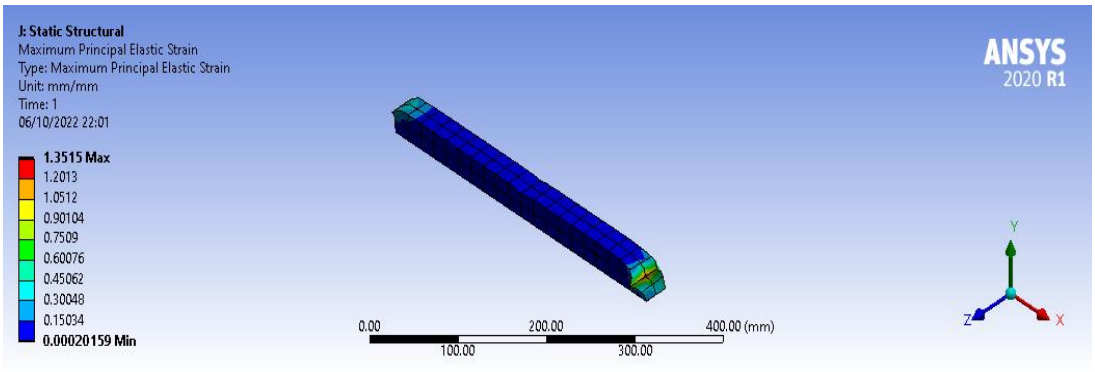

Fig-12 3-Point Bending Graphite Specimen Stress Formation

5.4. IMPACT TEST (IZOD)

The Izod Impact assessment was conducted to evaluate the impact resilience of the samples, which were fabricated in compliance with ASTM Standards. A consistent load of 78KN was directed onto the specimens, illustrating their strength upon the introduction of nano fillers, with the base held stationary. This test provided insight into the material's toughness and highlighted the overall deformation. The findings from the simulation are detailed below.

S.NO	Type of specimen	Impact Strength	Total Deformation
1	Control Composite	84656Mpa	346.9 mm
2	Graphite Composite	91533 Mpa	338.77 mm

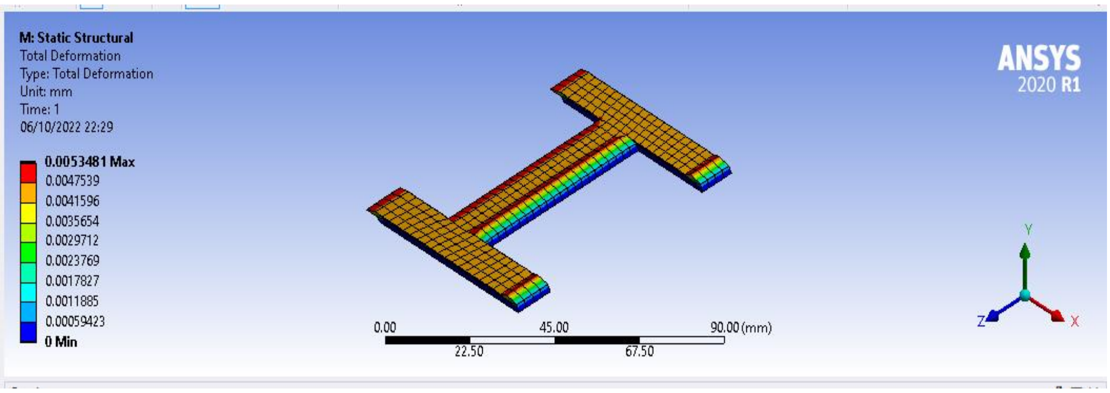

Fig-13 Impact Control Specimen Total Deformation

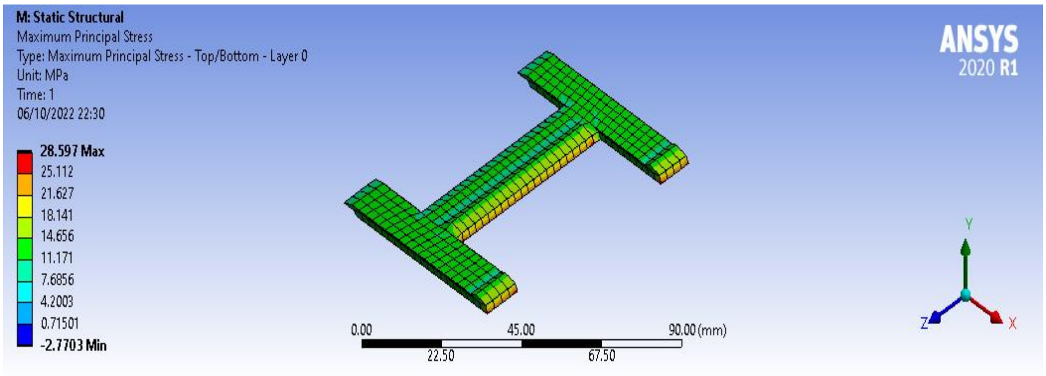

Fig-14 Impact Control Specimen Stress Formation

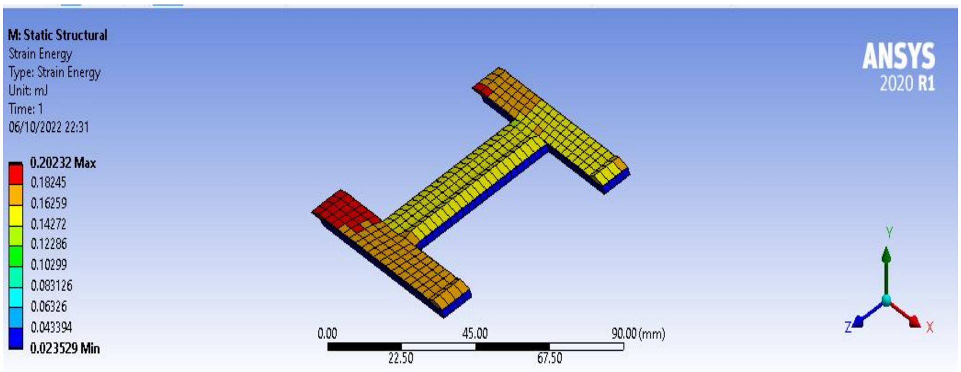

Fig-15 Impact Control Specimen Strain Analysis

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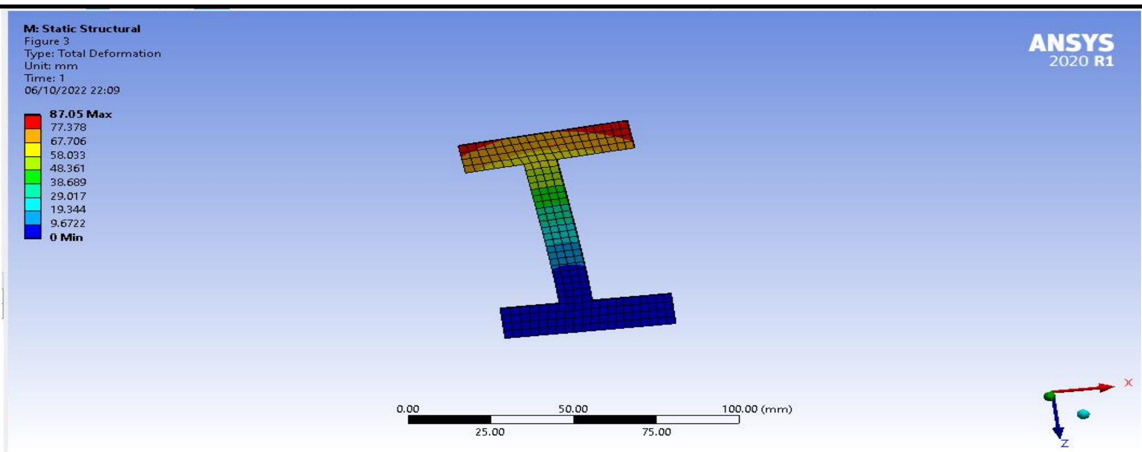

Fig-16 Impact Graphite Specimen Total Deformation

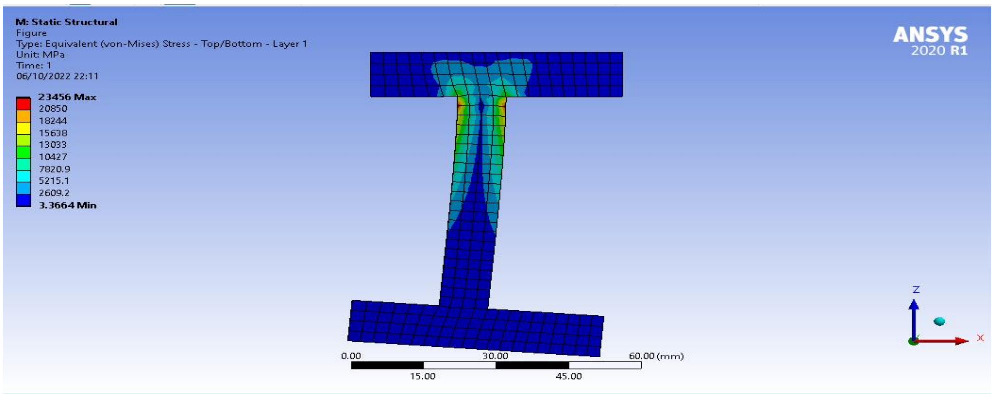

Fig-17 Impact Graphite Specimen Stress Formation

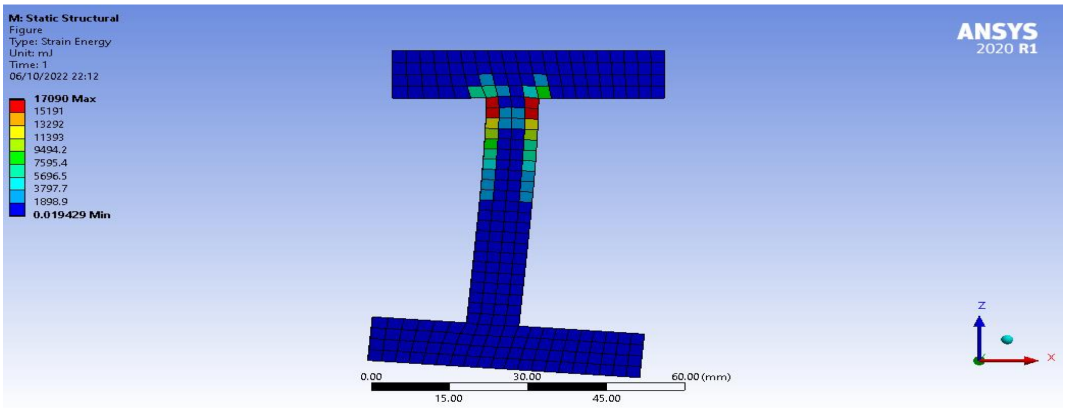

Fig-18 Impact Graphite Specimen Strain Analysis

5.5. HARDNESS TEST (BRINNEL'S)

The hardness test is carried out to determine the material's ability to resist deformation, revealing the connection between its hardness and other attributes. Given that the material weighs less than 1kg, the Brinell macro hardness test was employed, subjecting the material to a force of 78KN. The following observations were found from the software for Graphite dispersed Epoxy matrix composite reinforced with high silica fiber galss:

S.NO	Type of specimen	Deformation rate	Normal Stress	Strain Energy
1	Control Composite	4.679x10-2 mm	-0.32971 MPa	4.3957 MJ
2	Graphite Composite	4.1366x10-2 mm	-2.9989 MPa	5.0164 x 10-3 MJ

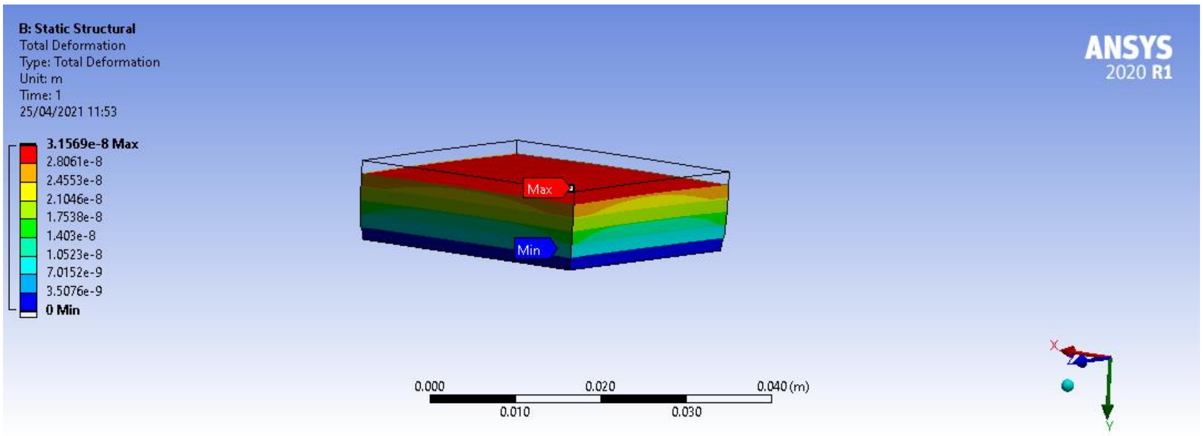

Fig-19 Control Specimen Total Deformation Analysis (Hardness)

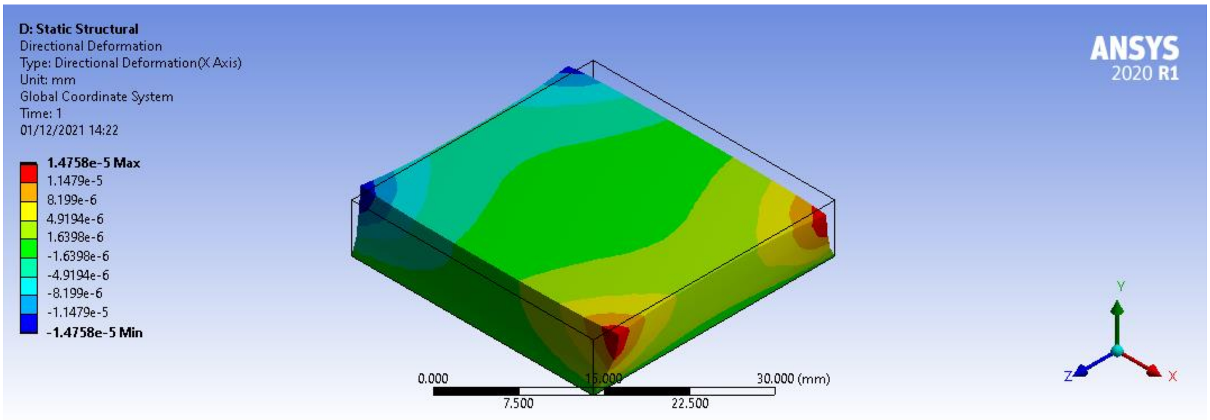

Fig-20 Graphite Specimen Total Deformation Analsysis (Hardness)

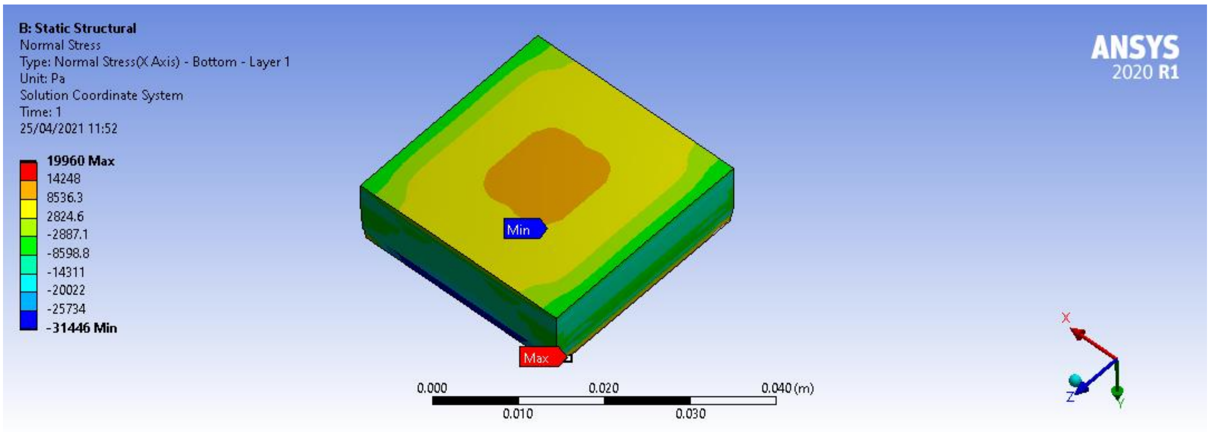

Fig- 21 Control Specimen Stress/Strain Analysis (Hardness)

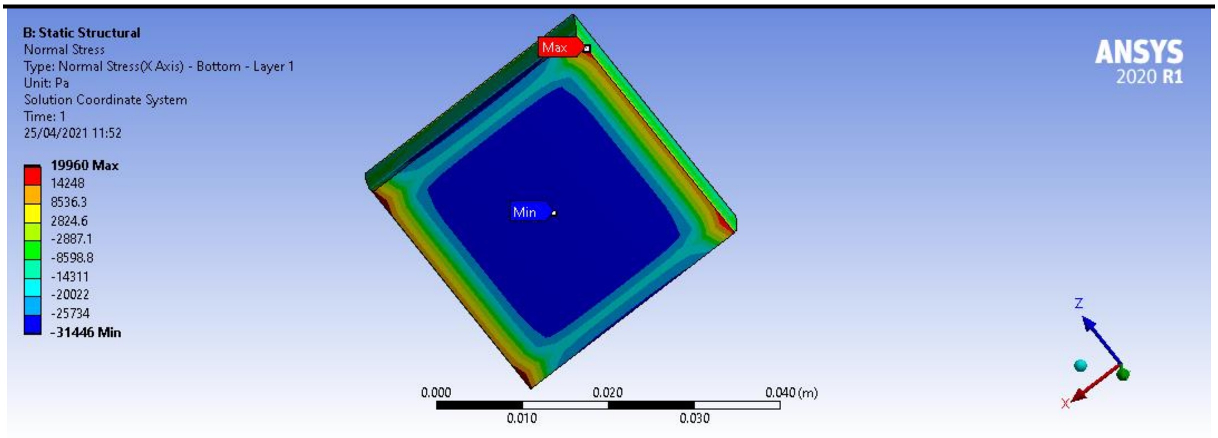

Fig- 22 Graphite Specimen Stress/Strain Analysis (Hardness)

5.6. THERMAL ANALYSIS

The examination was carried out to assess the thermal strength and heat flux of the material. The approach involved maintaining a consistent temperature on all surfaces of the sample while keeping it in a fixed position. Upon conducting the analysis, the following data was obtained for Graphite dispersed Epoxy matrix composite reinforced with high silica fiber glass:

Thermal Analysis Over Time			
	Temperature	Raw Specimen	Graphite
Minimum	3176.7 °C	4.3463e-004 W/mm²	2.4139e-003
Maximum	3176.7 °C	4.3463e-004 W/mm²	1.4048e-002

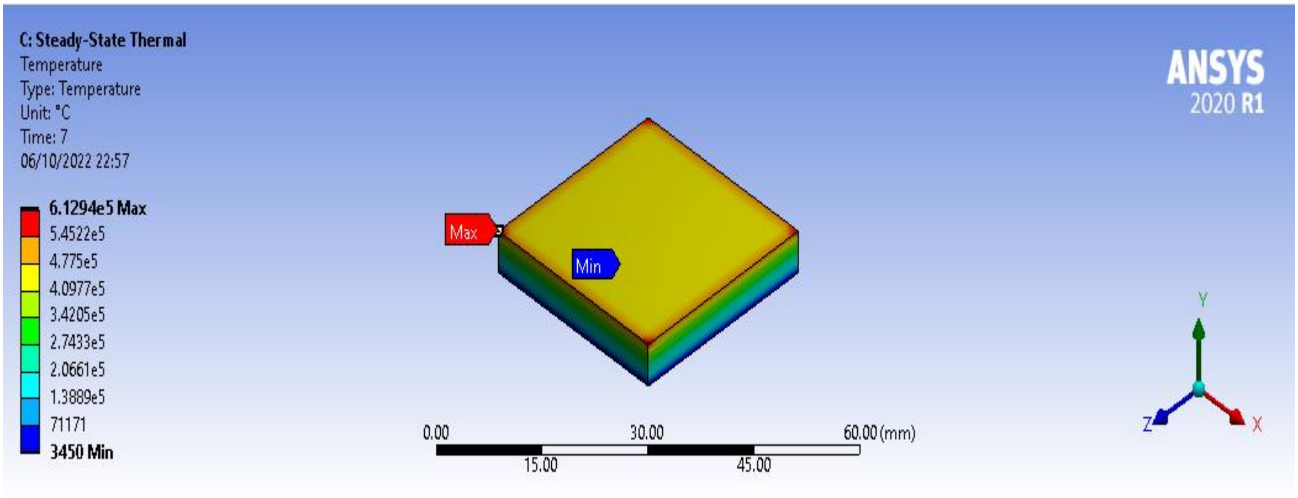

Fig-23 Control Specimen Thermal Analysis

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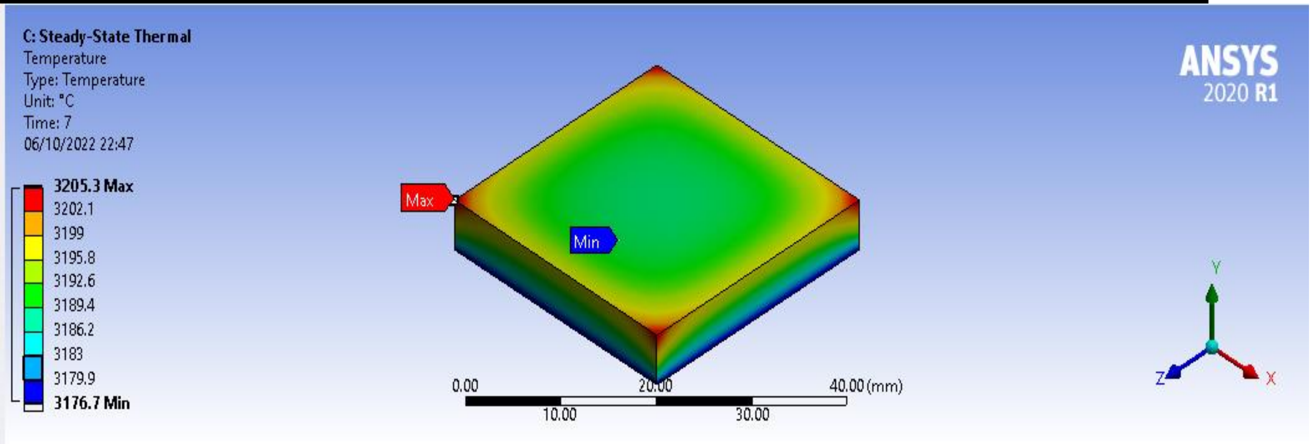

Fig-24 Graphite Specimen Thermal Analysis

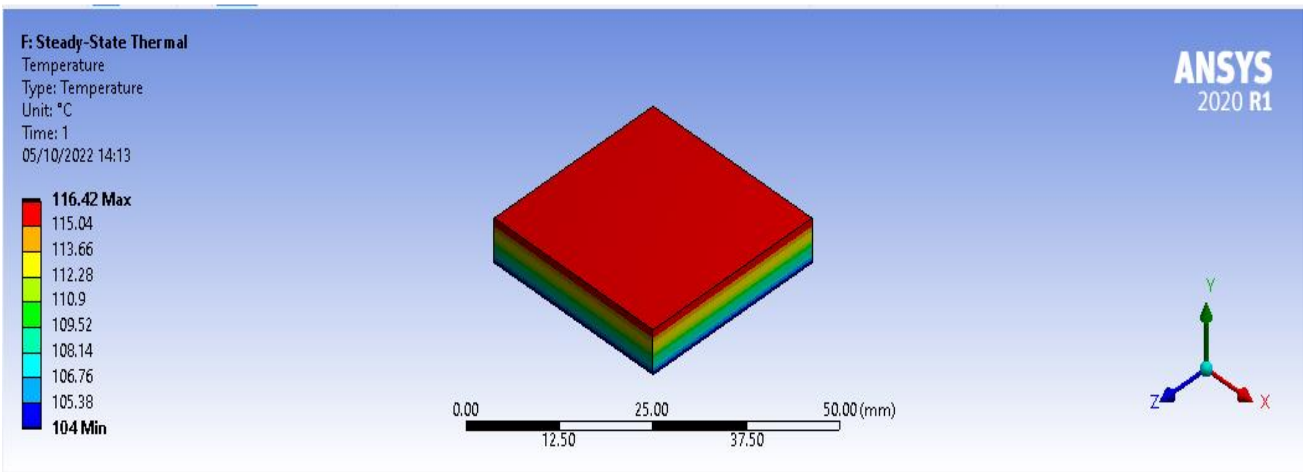

Fig-25 Graphite specimen Thermal Analysis (Hardness)

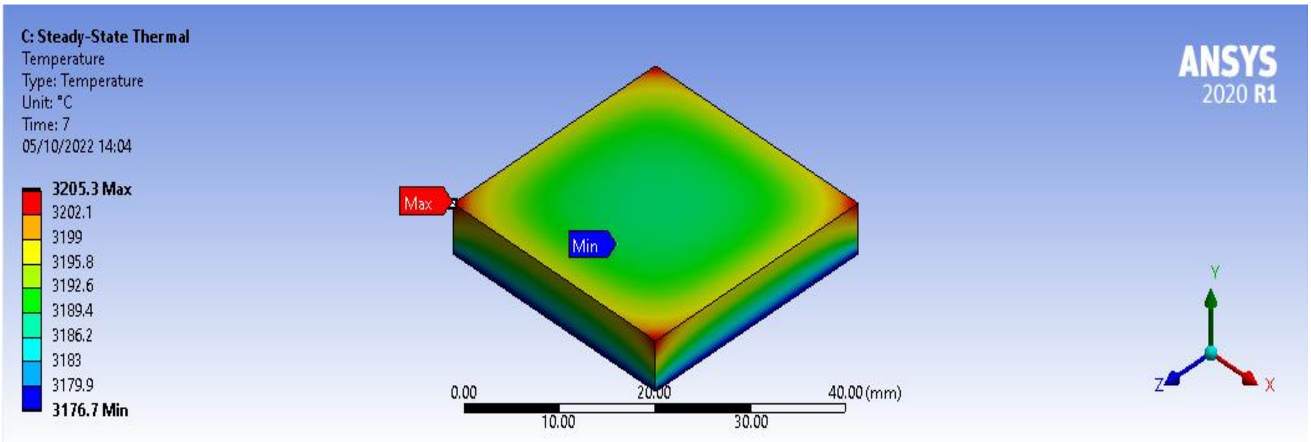

Fig-26 Graphite Tempreature /Heat Flux Analysis (Compression)

6. DISCUSSIONS ON THE RESULTS.

The results obtained can be expressed usingthe increase Vs decrase in strength, stress, strain and enery using the below table.

	Total Deformation	Normal Stress	Ultimate Tensile Strength	Elstic Strain	Energy
Compression	-	-	78% increase	-	-
Hardness	11% decrease	89% decrease	-	12% decrease	-
Tension	-	9% decrease	-	-	Equal amount of energy
Impact	2% decrease	-	8.1% increacse	-	-
3-Point Bending	31% decrease	2.2% decrase	-	51% decrase	-

Table: Final Analysis Comparison

The table above can be further expalined using the graph below.

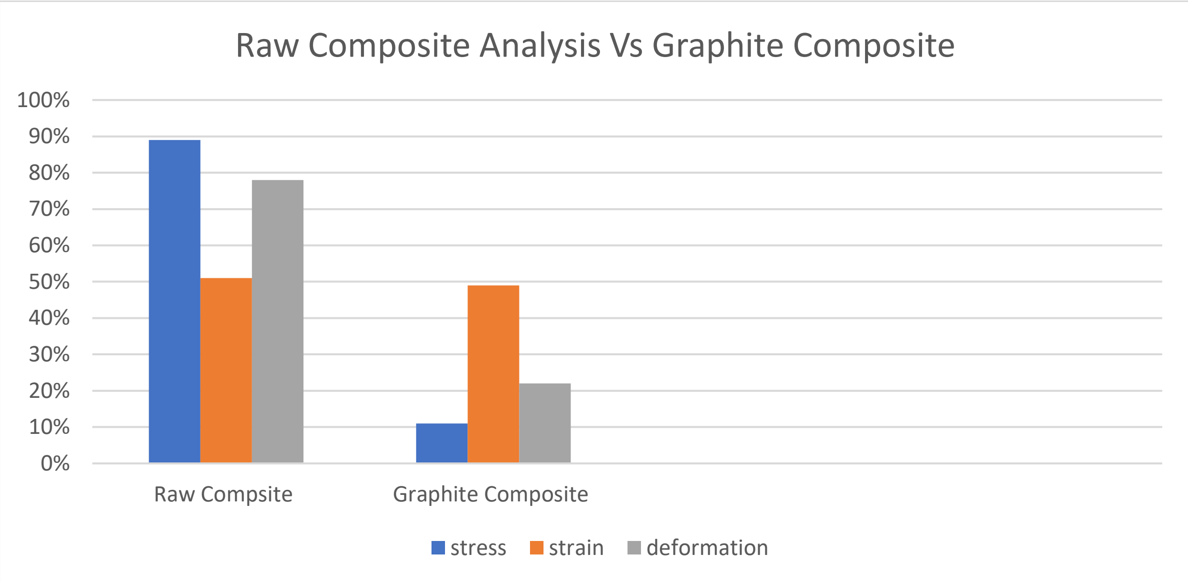

Chart-1 Raw Composite Analysis Vs Graphite Composite

The analysis sowcased that adding graphite nanofiller to highsilica fiber glass increased its strength and elsaticity rate, and decreased the deformation rate by decreasing the normal stresses and strain acting on the specimen. Adding graphite has increased the material strength by 70% and decreased the normal stresses and strain by 20 to 50%. Furthermore, the thermal analsysis showcased that the graphite specimen had a thermal strength higher than the raw specimen by 37%.

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