

ISTANBUL TECHNICAL UNIVERSITY ★ GRADUATE SCHOOL OF SCIENCE
ENGINEERING AND TECHNOLOGY

**THE EFFECT OF NANOTUBE INTERACTION ON THE MECHANICAL
BEHAVIOUR OF CARBON NANOTUBE FILLED NANOCOMPOSITES**

M.Sc. THESIS

Beril AKIN

Departement of Aeronautical and Astronautical Engineering

Aeronautical and Astronautical Engineering Programme

JANUARY 2012

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**Beril AKIN
511091158**

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Thesis Advisor: Assoc. Dr. Halit S. TRKMEN

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İSTANBUL TEKNİK ÜNİVERSİTESİ ★ FEN BİLİMLERİ ENSTİTÜSÜ

**NANOTÜP ETKİLEŞİMİNİN KARBON NANOTÜP İLE TAKVİYELİ
NANOKOMPOZİTLERİN MEKANİK DAVRANIŞINA ETKİSİ**

YÜKSEK LİSANS TEZİ

**Beril AKIN
511091158**

Uçak ve Uzay Mühendisliği Anabilim Dalı

Uçak ve Uzay Mühendisliği Programı

Tez Danışmanı: Doç. Dr. Halit S. TÜRKMEN

Ocak 2012

Beril AKIN, a **M.Sc.** student of ITU **Graduate School of Science Engineering And Technology** student ID 511091158, successfully defended the **thesis** entitled “*The Effect of Nanotube Interaction on the Mechanical Behaviour of Carbon Nanotube Filled Nanocomposites*”, which she prepared after fulfilling the requirements specified in the associated legislations, before the jury whose signatures are below.

Jury Members : **Prof. Dr. Zahit MECİTOĞLU**

Istanbul Technical University

Thesis Advisor : **Doç. Dr. Halit S. TÜRKMEN**

İstanbul Technical University

Doç. Dr. Halit S. TÜRKMEN

Istanbul Technical University

Doç. Dr. Hasan KURTARAN

Gebze Institute of High Technology

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To my mother and grandmother,

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Beril AKIN

Mechanical Engineer

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ABBREVIATIONS AND SYMBOLS

CNT	:Carbon Nanotube
CNTs	:Carbon Nanotubes
SWNT	:Single Walled Carbon Nanotube
SWNTs	:Single Walled Carbon Nanotubes
MWNT	:Multi Walled Carbon Nanotube
MWNTs	:Multi Walled Carbon Nanotubes
IUPAC	:International Union of Pure and Applied Chemistry
HRTEM	:High Resolution Transmission Electron Microscopy
THF	:Transparent Film Heaters
VdW	:Van der Waals
RVE	:Representative Volume Element
DOF	:Degrees of Freedom
PCG	: Preconditioned Conjugate Gradient Method

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THE EFFECT OF NANOTUBE INTERACTION ON THE MECHANICAL BEHAVIOUR OF CARBON NANOTUBE FILLED NANOCOMPOSITES

SUMMARY

In aeronautical structures, secondary loads have critical effect on the stability of the structure. In this instance, nanoreinforcement of anisotropic materials makes ameliorations to their directional deficiencies. Carbon nanotubes are a well-known strengthening particulate in nanocomposites. In a carbon nanotube-polymer system, carbon nanotubes often have a slight curvature and can be mechanically in contact at nanoscale with each other within the polymer matrix material.

The research objective includes the effect of mechanical contact interaction between two carbon nanotubes, to the global response of material. It is a carbon nanotube reinforced polymer system. Carbon nanotube is a filler material within an epoxy matrix constituting a nanocomposite system. An actual technique of modeling nanocomposites namely, square representative volume element is used. The model contains epoxy and nanotubes with a perfectly bonded interface assumption. Two different waviness ratios are studied. Carbon nanotubes are initially in contact between each other. The model is symmetric and subjected 20 nm displacement in compression. The representative volume element is modeled via the finite element method. The carbon nanotube is modeled by considering to be a shell structure of 0.34 nm thickness. The curvature of carbon nanotube is considered as a sinusoidal function modeled via Matlab® and Ansys® Parametric Design Language. The analysis of the representative volume element is achieved with and without contact with each other of nanotubes.

Elastic modulus obtained by rules of mixtures using the filler volume fraction where contact and waviness effect are not included, is 5.12 GPa. It is 1-2% higher than the elastic modulus of with and without contact cases with two different waviness ratios. Thus, it can be said that, while waviness ratio increases, the global elastic modulus decreases.

Additionally, for the model which carbon nanotubes have 0.2 waviness ratio results %0.3 stiffness contribution to the global elastic modulus observed due to mechanical contact effect. It can be said that interaction of carbon nanotubes has a strengthening effect in carbon nanotube filled nanocomposite.

NANOTÜP ETKİLEŞİMİNİN KARBON NANOTÜP İLE TAKVİYELİ NANOKOMPOZİTLERİN MEKANİK DAVRANIŞINA ETKİSİ

ÖZET

Uçak yapılarında, kompozit malzemelerin kullanımı hafiflik ve dayanım gerekliliğinden dolayı kaçınılmazdır. Ancak izotropik olmayan malzemeler, takviye yönüne aykırı doğrultulardan gelen yüklemelere karşı zayıftır ve bu durum yapıda kararsızlıklara sebep olabilmektedir. Bu sebeple gelişen malzeme teknolojisi ile uçak yapılarında nanomalzemelerden faydalanılmakta yapıların dayanımı ve kararlılığı arttırılmaktadır. Karbon nanotüpler, günümüzde popüler takviye elemanlarıdır ve polimer matris içerisinde yapısal ya da fonksiyonel amaçlı kullanılmaktadır.

Özellikle karbon nanotüp ihtiva eden nanoelektromekanik malzemelerde, enerji depolama, bilgi işleme uygulamalarında karbon nanotüplerin birbirleriyle etkileşimlerinden faydalanılmaktadır. Nano ölçekteki yapıların atomsal ölçekteki etkileşimleri sayesinde birçok yeni malzeme üretilmekte, var olan malzeme konseptleri değişmektedir. Fakat makro ölçekte de örneğin karbon nanotüp takviyeli polimerlerde de matris fazı içerisinde dağılmış karbon nanotüpler arasında oluşan elektriksel, termal veya mekanik kontak etkileşimlerinin malzemenin fiziksel ya da mekanik davranışına etkisi bulunmaktadır.

Karbon nanotüpler polimer matris içerisinde, kavisli şekillerde ve birbirleriyle mekanik olarak ilişkili pozisyonlarda bulunabilmektedir. Bu tezde, epoksi matris içerisinde birbirine paralel konumlanmış belli kavis değerlerindeki karbon nanotüplerin birbirleri arasındaki mekanik etkileşimlerinin, malzemenin genel elastisite modülüne etkisi bir yapısal model kurularak incelenmiştir.

Çalışmada karbon nanotüp takviyeli epoksi matrisli nanokompozit, ara yüzü mükemmel yapışma kabulü ve simetrik sınır değerler verilerek oluşturulmuş temsili birim eleman metodu ile modellenmiş ve sonlu elemanlar yöntemi ile incelenmiştir. Model Matlab® yardımı ile kurulup Ansys®'e Parametrik Tasarım Dili yardımı ile aktarılmıştır.

Karbon nanotüpler 0.34 nm kalınlığında kabuk eleman olarak modellenmiştir. Matris fazı ise epoksi malzemeden olup, solid eleman kullanılmıştır. Matris ve karbon nanotüpler arasında mükemmel yapışma olduğu kabul edilmiştir. Yüzeyler arası sürtünme katsayısı, iki karbon yüzey arası sürtünme katsayısı yaklaşık olarak, 0,1 olarak alınmış ve karbon nanotüplerin yüzeyleri pürüzlü kabul edilmiştir çünkü sürtünme dışında da atomlar arası etkileşimler, Van der Waals bağları ya da kimyasal

bağlar mevcuttur. Kontak Gauss yüzeyleri üzerinde tanımlanmış, integrasyon nodlarının artırılması amacıyla 4-node shell 181 tipli eleman tam integrasyon ile kullanılmıştır. Sürtünme katsayısı düşük olduğundan simetrik matris kullanılmıştır. Kontak modeli, penetrasyon limitlerinin belirtilmesini sağladığından, Artırılmış Lagrange çarpanları algoritması ile çözdürülmüştür. Shell elemanın yönelimi 0 derece, yani açısızdır. Analiz statiktir, kontak modelinden dolayı doğrusal değildir. Doğrusal olmayan denklemlerin derecelerini daha fazla arttırmamak için küçük deformasyon kabulü yapılmış ve 2 alt adımda kontaklı modellerde PCG diğerlerinde ise kontak algoritmalarıyla daha uyumlu olması açısından frontal solver kullanılarak çözdürülmüştür.

Sonuç olarak, mekanik kontak etkisi, başlangıçta birbirlerine değen ve değmeyen yüzeyler arasından hesaplanmış ve mekanik kontak etkisinin ihmal edildiği modellerle birlikte her bir kavis değeri için ayrı ayrı hesaplanmıştır. Modelde bası yönünde statik yükleme verilmiştir. Yükleme birbirlerine başlangıçta değmeyen karbon nanotüp konfigürasyonunu içeren modellerde her durum için farklı ve birbirine değen yüzeylerle oluşturulmuş kontak modelleri içeren durumlar için ise üniform bir değer kullanılmıştır.

Karbon nanotüplerin elastik modüllerinin 1 GPa ve epoksi elastik modülünün 5 GPa olarak kabul edildiği modelde. Modelin hacim oranından yola çıkarak ve karbon nanotüplerin kavisli formları ihmal edilerek uygulanan karışım yasasına göre genel elastisite modülü 5.12 GPa'dır. Bu değer modellerde bulunan değerlerden %1-2 daha yüksektir. Kavis oranının ihmal edildiği için bu beklenen bir değerdir.

Ayrıca 0.2 kavis oranına sahip karbon nanotüp içeren modelde mekanik kontak etkisinin malzemenin genel elastik modülünü %0.3 oranında arttırdığı gözlenmiştir. Bu sonuçtan yola çıkarak, kontak etkisinin malzemenin genel elastisite modülünü artırıcı yönde etki ettiği söylemek mümkündür. 0.3 kavis oranına sahip karbon nanotüp içeren modelde ise, modelde oluşmuş zorluklardan dolayı kontaklı ve kontaklı modeller arasında değerlendirme yapılamamıştır. Bu karşılaştırmaların sayısal değerlerinden yola çıkarak, iki farklı kavis değerine sahip modellerde genel elastisite modülü kavis oranı arttıkça, literatürde bahsedildiği gibi azalmaktadır.

İki karbon nanotüp arasında 1 nm boşluk içeren konfigürasyonda ise, kontak modellemede zorluk yaşanmış, bundan dolayı sonuçlar değerlendirmeye alınmamıştır.

Sonuç olarak, çeşitli konfigürasyonların denenmesiyle yalnızca birbiriyle paralel ve değen iki yüzey arasındaki etkileşimin olduğu model değerlendirilmiştir. Varılan en önemli sonuç, mekanik kontak etkisinin birbirlerine paralel doğrultularda yönelmiş carbon nanotüp içeren bir epoksi matrisli nanokompozit yapının elastisite modülünü arttırdığıdır. Sonuçlar henüz deneysel bir çalışma ve istatistiksel bir yaklaşım ile doğrulanmamıştır.

Gelecek alıřmalarda, bu model temel alınarak atomsal etkileřimlerin de ihmal edilmedięi ok lekli bir model elektriksel kontak etkisini de ierecek řeklinde oluřturulup incelenecektir.

1. INTRODUCTION

Composite materials are integrated units composed of different constituent phases, which are chemically dissimilar. In other words, they are multiphase materials artificially produced to obtain favorable properties. Actually, recent technology needs new materials exhibiting high performance. For conventional materials, a trade-off must be made between some properties especially, stiffness and weight or toughness and brittleness. However, composites can be tailored for technological requirements by changing their component's types, proportions, configurations, morphologies, degrees of crystallinity...etc. Composites can also be found also in nature; the most known examples are bone and wood.

The way of searching for high-performance materials gives birth to composite material technology of today but this motivation dates earlier. Ancient Egyptians used a composition of clay and straw as a structural reinforcement for strengthening their buildings.

The mixture of a matrix with filler in the nanometer scale gives the name "nanocomposite" where the first application is reported by the Toyota research group on a Nylon-6/motmorillonite (N6/MMT) blend that was used on a timing belt cover (Okada & Usuki, 2006). Nanofiller reinforced polymer composites gained enormous interest in this last decade. They provide lightweight, strong, flexible and resilient structures. As filler materials, polymer matrix nanocomposites can involve; clay, carbon nanotube, carbon nanofillers, graphene, and inorganic nanofillers...etc. The main fields where nanocomposites are in use: Polymer reinforcements, flame resistances, electro-optics, biotechnology...etc. Polymer nanocomposites can be classified as structural nanocomposites and functional nanocomposites. For structural nanocomposites, mechanical superiorities such as stiffness, rigidity, flexibility, strength, weight are required; while for functional nanocomposites physical properties such as electrical or thermal conductance are important.

1.1 Motivation

Nanocomposites by means of nanoreinforcement resolve structural problems due to anisotropic behavior of conventional reinforcement. For example, the upper wing of an aircraft usually subjects uniform compressive loads. However, under the unfavorable weather conditions, secondary loads in transverse directions may occur. For anisotropic materials, subjecting torsion along the poorly reinforced direction may cause flight instabilities. This is the major drawback of composites in aeronautics. However, use of lighter materials is indispensable for weight reduction in aeronautics. This challenge ultimately affects the material science evolution of today, leading the use of nanomaterials in aeronautical structures.

Actually a commercial application of nano reinforcement can be found in tennis balls Double Core™ balls of Wilson which has been recently official balls for Davis Cup have vermiculite platelets exfoliated and aligned within the butyl rubber. The multi-layer of the platelets acts as diffusion barriers while rubber phase gives flexibility. They retain original pressure and bounce twice compared to the conventional balls (Callister, p.612-613).

Besides, memory chips are an example of the use of carbon nanotubes. There are memory chips using contact resistance property for a random-access memory design as in the (Url-2). In this example, the contact of the carbon nanotubes is representing with “1” state and the non-contact state is representing with “0” state. Ensuring a logic configuration using carbon nanotubes in contact with each other.

Carbon nanotubes have spring-like properties as indicated by (Chesnokov et al., 1999) are using for energy storage mechanisms.

1.2 Problem Statement and Research Objectives

In a carbon nanotube reinforced polymer system, carbon nanotubes can be mechanically in contact with each other. The mechanical effect of this interaction at a global level is the subject of this thesis. Research objectives include representative volume element modeling of a two carbon nanotubes having a specific waviness and the mechanical interaction between them in a defined gap. The study is driven with different waviness ratios. In order to make a comparison, all models are studied with and without contact.

1.3 Literature Review

Carbon nanotubes is the stiffest material ever made having a Young modulus between the range of 1 to 5 TPa (Lijima, 1991). A tensile strength about 100-600GPa (Cooper et al., 2002) and density about 1.8-1.9g/cm³ (Collins, 2000). Although their extreme high stiffness carbon nanotubes are flexible structures, which can resist to twist, buckling, and they can be deformed reversibly without breaking (Lijima, 1996).

1.3.1 Carbon nanotubes

Carbon is an element which has a variety of utilization known since 5000BC. While the main element of organic compounds, carbon is classified in 1807 by Berzelius, who defined that carbon as the main element in organic substances. Afterwards by J. Van t'Hoff H. and Le Bel J.A. suggest the configuration of carbon atom as tetrahedral. The element compositions found by King A.S and Birge R.T. from the isotopes C¹² and C¹³ in 1929. In 1936, radioactive C¹⁴ was detected by Burcham W.E. and Goldhaber M. The radiocarbon dating for the age determination of the organic materials is discovered by Libby and awarded for Nobel's prize in 1960. One year further, C¹² was established as a basis for the standard atomic masses (C¹²=12000 cmu). The invention of C¹³ Fourier Transforms for spectral analysis help to investigate studies on organic molecules as explained in (Krueger, p.2-3).

Carbon is constituting many polymorphic formulations. One of them is the Buckminsterfullerenes or fullerenes shortly Bucky's ball (C₆₀), which is discovered in 1985 by (Smalley R.E., 1985). The history of the discovery of Buckminsterfullerenes starts from Smalley and Curl, when they developed a technique to analyze atom clusters in september 1985. In 1990, Smalley proposed the existence of a tubular fullerene. Multi-walled carbon nanotube is discovered by (Lijima, 1991) via a transmission electron microscope. But carbon nanotubes are firstly, observed in 1956 by (Bacon, 1960).

By definition, a carbon nanotube (single-walled) is a rolled-up graphite sheet having 10 to 20 C-C bonds per repeat unit. The C-C bond is among the strongest bond in the universe; the elastic modulus of carbon nanotube is on the order of 1 TPa, near to diamond, and 3-4 times greater than carbon fiber. The tensile strength is in the range

of between 200-500 GPa and fracture strains between about 5-20% (Callister, p.433). However, these values are much lower in practical uses due to structural defects.

The carbon atom has six electrons with the configuration of $1s^2 2s^2 2p^2$ in the ground state. The electron in s orbital promotes to p orbital and atom are said to be an excited state. Afterwards, electrons reorganize themselves into identical hybrid orbitals, called hybridization. sp hybridized C atoms form linear chains, whereas sp^2 and sp^3 hybridization gives rise to planar structures and to three-dimensional networks. In sp or sp^2 hybridized atoms, there are two or one p atoms, which are outside of the hybridization process, can form π -bonds. The overlap between two C atoms forms σ bonds. Chiral vectors (n,m) can be expressed as,

$$C_h = n\hat{a}_1 + m\hat{a}_2 \quad (1.1)$$

Where $\hat{a}_1$ and $\hat{a}_2$ are two basis vectors and n and m are the chiral angle;

$$\theta = \tan^{-1}[\sqrt{3}(n/(2m+n))] \quad (1.2)$$

Having a value in the range of $0^\circ \leq \theta \leq 30^\circ$, which is the angle between C-C bonds and tube's axis. The tube is called chiral tube. In zig-zag tubes, $n \neq 0$, $m=0$ meaning C-C bonds are paralelel with the carbon nanotube axis while in the armchair tubes, $n=m \neq 0$ the C-C bonds are perpendicular to the carbon nanotube as explained in (O'Connell, p.6-8). The chirality, directly influence the physical and mechanical properties of the carbon nanotube (eg.the fracture behavior of carbon nanotube, in onder words on the ductlity or brittleness) as explained in (Nardelli et al.,2000).

For the aim of improving carbon nanotube dispersions in the polymer matrix, creating better bonding with the polymer matrix, increasing the carbon nanotube solubility in solvents and facilitating carbon nanotubes to form a network the most-recent method is the chemical functionalization, is applicating. The logic is the creating chemical covalent bonds between the carbon nanotube and the polymer.

Another suggestion, carbon nanotubes are not straight practically within the composite, this decrease the global modulus of the composite (Fisher et al., 2002).

A small amount of carbon nanotube into a highly crystalline thermoplastic polymer matrix can increase the elastic modulus in more than 100% (Coleman et al., 2006). For a carbon nanotube reinforced epoxy polymer systems 1.5 wt.% nanotube content make 17% increase of elastic modulus as expressed by (Song & Youn, 2005).

Carbon nanotube based nanocomposites are in general using as electrostatic discharge (ESD) materials in various fields. According to Zhao et al.,(2001), it is explained with the Raman spectrum of carbon nanotube. by monitoring the D* band at 2610cm^{-1} in the air, which is sensitive to its strain rate, carbon nanotubes can be used as strain sensors in polymers Nanotubes could be embedded in high-performance composites as reinforcing material and can be used as strain sensors allowing nanodestructive health monitoring capability for structures.

1.3.2 Carbon nanotube filled nanocomposite

Thermosetting materials are often liquid materials after curing through heat, chemical agents or radiation. 3D networks are formed by cross linking polymer chains together and forms an irreversible state. Mechanical properties depend on the density and length of these polymer chains. Thus, they have better properties to environmental stress, to crack or to creep than many thermoplastics.

According to the definition of IUPAC, (2007): “A thermosetting polymer is a prepolymer in a soft solid or viscous state that changes irreversibly into an infusible, insoluble polymer network by curing.”

Thermosetting polymers are cured and become in an irreversible state called thermoset (Url-3). At the beginning of the curing process, thermoset polymers are telechelic reactive oligomers containing two or more components. Solidification begins when oligomers react with hardener and ambient temperatures. Subsequently, a rigid or highly crosslinked network (or vitrified system) is formed (Akovalı, p.25). This process of curing is also called as polymerization. The main advantages that epoxy thermosets have are; low shrinkage, good control of crosslinking and availability of ranging from low to high viscosity (Ratna, p.4-5).

Epoxy resin is most commonly used matrix polymer for composites as well as nanocomposites. A high temperature thermoset matrix, consist of epoxide groups, which are formed with one oxygen and two carbon atoms.

Epoxy have a tensile strength of 103 MPa, an elastic modulus of 3.4 GPa, a ductility (elongation at break) of 6%, and a density of 1.25g/cm^3 , according to (Askeland & Phule, p.597).

Nanocomposites are composites, which have components smaller than 100 nm (Gupta et al., 2010). The challenge of nanocomposite is to engineering atoms such that materials and devices have new mechanical, chemical, electrical, magnetic or optical properties.

Nanocomposite technology history begins with exfoliated clay reinforcement in polymer system. The first nanoclay-polyamide system is introduced by (Okada & Usuki, 1995). The first commercial application is introduced by Toyoto in its timing belt covers in 1993 (Gupta et al., p.2). which is the first commercial use of polymer based nanocomposite. After the discovery of carbon nanotube in 1991, a new era is started for nanocomposite material technology. Materias having superior mechanical properties are introduced.

According to Ajayan et al., (2000) the strength of a single walled carbon nanotube-polymer composites can be improved by disperison of individual carbon nanotubes inside the polymer material (not to use carbon nanotubes in bundles) and chemically crosslinking carbon nanotubes with each other.

Carbon nanotubes are not soluble into the solvents, thus dispersing them homogeneously is difficult. There are several methods for improving bonding capabilities of carbon nanotubes. First one is the chemical strengthening of the nonbonded interactions with the nanotube (e.g by wrapping a large polymer molecule around the nanotube). The other one is the forming chemical covalent bonds between the nanotube and the polymer directly, also known as functionalization explained by (Odegard et al., 2003).

1.3.3 Load transfer mechanisms

The carbon nanotube-polymer interface is the most critical zone in the material. If the adhesion of the carbon nanotube and polymer interface is strong enough composite can maintain under higher stress values without damage. The interfacial shear stress between the fiber and the polymer affect the load transfer mechanism. There are mainly three mechanisms, according to (Bal & Samal, 2007).

1.3.3.1 Micromechanical interlocking

This load transfer mechanism occurs in many fibers due to defects on the surface of the fiber. The atomic structure in carbon nanotubes have any or few defects and that's why micromechanical interlocking is not a load transfer mechanism for nanocomposites.

1.3.3.2 Chemical bonding

Ionic or covalent bonds are formed in the interface which facilitates the load transfer.

1.3.3.3 Weak Van der Waals bonding

It occurs by Van der Waals bonds between carbon atoms. It's the most common mechanism for interfacial load transfer and the main interaction mechanism of carbon nanotubes.

2. MODELING OF THE REPRESENTATIVE VOLUME ELEMENT

Heterogeneous material analysis is carried out by homogenisation techniques, which simplify the calculation process. Unit volume of the material is analysed in order to calculate the whole system. This volume is often called representative volume element or unit cell which as the name suggests represents the whole geometry, boundary conditions and the loading applied.

2.1 Modeling of the Representative Volume Element

Material modeling methods consist of computational chemistry, multiscale modeling and computational mechanics. Material modeling in a length scale of one angstrom to one meter consist of quantum mechanics, nanomechanics usually use discrete domain assumption and micromechanics, structural mechanics use continuum domain assumption.

The computational methods used on chemistry are generally used to compute atomic interactions, chemical reactions between the carbon nanotube and polymer material...etc. While computational mechanics generally use continuum approach, which gives useful global responses of nanocomposite, individually carbon nanotubes, load transfer mechanism, effective stiffness deformations...etc.

The influence of nanotube agglomeration on the effective stiffness analyzed by a micromechanical model developed and found that it reduces global stiffness of the material by (Dong-Li Shi et al., 2004).

For a good mechanical and structural performance, it's necessary that interfacial shear strength must be high. However, for functional nanocomposites, the contact resistance between carbon nanotubes must be low in order to achieve thermal or electrical conductance (Bal & Samal, 2007).

In this study, square representative volume element method as shown by (Chen & Liu, 2004) is used and a representative volume element containing two carbon nanotube and epoxy component is modeled.

2.2 Modeling of Carbon Nanotube-Polymer Interface

Interface region between carbon nanotube and matrix has critical importance for effective load transfer mechanism. For simplifying the simulations, interface can be assumed perfectly bonded, which is demonstrated by researchers (Jia et al., 1999; Thostenson et al., 2001).

Carbon nanotube based nanocomposite fracture have brittle behavior (Mai & Yu, p.348). Splitting of carbon nanotube bundles, kink formation in the carbon nanotube bundle are possible damage modes and carbon nanotube fatigue failure mechanisms at the nanometer level shown by (Mai & Yu, p.348).

Carbon nanotubes can be considered as short fibers and the interaction between the carbon nanotube and the matrix can be explained by Cox (Shear Lag) theory as explained by (Chen et al. 2011).

The matrix and carbon nanotube are assumed elastic and perfectly bonded with each other. Elastic stress transfer between carbon nanotube and matrix without considering slip or yield can be modeled basically from stress equilibrium where interfacial shear force and axial stress can be calculated via;

$$\pi r^2 d\sigma = -2\pi r dx \tau \quad (2.1)$$

Where σ is the stress along the carbon nanotube, τ is the interface shear stress, x is the coordinate along the length of carbon nanotube.

For elastic transfer, after integrations;

$$\frac{d^2\sigma}{dx^2} - \beta^2\sigma = -\beta^2\sigma_\infty \quad (2.2)$$

The fiber stress is changing from σ_f to $\sigma_f + d\sigma_f$ along an element of length dx . Where β is shear-lag parameter, σ_∞ is the far-field fiber stress and σ is fiber stress.

The stress distribution along the carbon nanotube is,

$$\sigma = E\varepsilon[1 - \cosh(\beta x)\operatorname{sech}(\beta x)] \quad (2.3)$$

Where the shear-lag parameter,

$$\beta = \frac{1}{r} \sqrt{\frac{2G_m}{E \ln(s/r)}} \quad (2.4)$$

G_m is the matrix shear modulus, E is the elastic modulus and the average distance between the carbon nanotubes axes (Mishnaevsky, p.69-71),

$$s = (l_e - l_b) / r_{NT} \quad (2.5)$$

l_e : The total length of the tube, l_b : Bonded length

The shear stress alternation is obviously affected by interface behaviour problems such as slip, debonding....etc.

2.3 Modeling of the Contact

Contact modeling formulation can be done via mechanics of materials and continuum mechanic's principles and focuses on interactions between bodies as pressure, stress, friction and adhesion. Contact type of constraint is occurring in many engineering applications as well as deformation of composite material's constituents.

2.3.1 Analytical contact modeling

Assuming bodies B^α with boundaries Γ_c are contacting with each other during a finite deformation. The initial coordinates of the points $\mathbf{X}^1$ and $\mathbf{X}^2$ are different while after a finite deformation, contact occurs and the coordinates coincided. The contact phenomenon can be described with the coordinates of points $\mathbf{X}^1$ and $\mathbf{X}^2$ with the time, t ;

$$\varphi(\mathbf{X}^2, t) = \varphi(\mathbf{X}^1, t) \quad (2.6)$$

In the case of linear elasticity, the equilibrium condition can be described as,

$$-\text{Div} \boldsymbol{\sigma} = \mathbf{f} \quad \text{in } B \quad (2.7)$$

And the strain field $\boldsymbol{\varepsilon}$ is,

$$\boldsymbol{\varepsilon}(\mathbf{u}) = \frac{1}{2} (\text{grad} \mathbf{u} + \text{grad}^T \mathbf{u}) \quad (2.8)$$

The Hook law,

$$\boldsymbol{\sigma}(\mathbf{u}) = \mathbf{E}\boldsymbol{\varepsilon}(\mathbf{u}) \quad (2.9)$$

Where $\mathbf{E}$ is the elasticity tensor, and $\mathbf{u}$ is the displacement field. Boundary conditions existing on the body can be as follows,

1. Dirichlet Condition

$$\mathbf{u} = \mathbf{0} \quad \text{on } \Gamma_u \quad (2.10)$$

2. Neumann Condition

$$\boldsymbol{\sigma} \cdot \mathbf{n} = \mathbf{t} \quad \text{on } \Gamma_\sigma \quad (2.11)$$

3. Contact Condition

$$u_N - g \leq 0 \quad (2.12)$$

$$p_N \leq 0 \quad \text{on } \Gamma_u \quad (2.13)$$

$$(u_N - g)p_N = 0 \quad (2.14)$$

Where $\mathbf{n}$ is the outward normal of the surface of the solid and $\mathbf{t}$ denotes applied traction on Γ_σ as shown by (Wriggers, p.94-95).

Let $\mathbf{u}$ is a solution of the problem introducing in the weak form;

$$\int_B \boldsymbol{\sigma} : \boldsymbol{\varepsilon}(\mathbf{u} - \mathbf{v}) dV = \int_B \mathbf{f} \cdot (\mathbf{u} - \mathbf{v}) dV + \int_{\Gamma_\sigma} \mathbf{t} \cdot (\mathbf{u} - \mathbf{v}) d\Gamma_\sigma + \int_{\Gamma_c} p_N(\mathbf{u})(u_N - v_N) d\Gamma_c \quad (2.15)$$

$\boldsymbol{\sigma} = \boldsymbol{\sigma}(\mathbf{u})$ is a function of the displacement, $\mathbf{f}$ is the body force and $\mathbf{t}$ denotes the boundary traction as shown by (Wriggers, p.94-95).

The total potential energy of the elastic body consists of the total of the elastic strain energy U , and the potential energy V of the applied forces:

$$\Pi = U + V \quad (2.16)$$

The principle of minimum total potential energy can be expressed as,

$$\delta \Pi = \delta (U + V) = 0 \quad (2.17)$$

Expressing the constituents with virtual work principle the equality becomes,

$$\delta\Pi = \int_V \boldsymbol{\sigma}^T \delta\boldsymbol{\varepsilon} dV - \int_V \mathbf{f} \delta\mathbf{u} dV - \int_A \mathbf{t} \delta\mathbf{u} dA + \delta\Pi_c \quad (2.18)$$

Contact contribution to the weak form for the body in contact can be described by several ways but Lagrange multiplier method is the interest of this thesis.

2.3.1.1 Lagrange multiplier's method

The contact contribution Π_c can be formulated as follows;

$$\Pi_c = \int_A (\lambda_N \mathbf{g}_N + \lambda_T \cdot \mathbf{g}_T) dA \quad (2.19)$$

Where λ_N and λ_T are the Lagrange multiplier, $\mathbf{g}_N$ and $\mathbf{g}_T$ are the normal and tangential gap functions. The variation of Π_c ;

$$\delta\Pi_c = \int_A (\delta\lambda_N \mathbf{g}_N + \lambda_T \cdot \delta\mathbf{g}_T) dA + \int_A (\lambda_N \delta\mathbf{g}_N + \delta\lambda_T \cdot \mathbf{g}_T) dA \quad (2.20)$$

Lagrange multiplier λ_N can be identified as the contact pressure $\mathbf{p}_N$. $\delta\mathbf{g}_N$ is the variations of the normal gap. The terms $\lambda_T \cdot \delta\mathbf{g}_T$ and $\delta\lambda_N \cdot \mathbf{g}_N$ are associated with the tangential stick. λ_N is as a “force” applied to each other to prevent penetration. The gap condition between bodies, B^α can be shown as,

$$\mathbf{g}_N = \mathbf{g} - (\mathbf{X}^2 - \mathbf{X}^1) \cdot \mathbf{n}^1 \quad (2.21)$$

where $\mathbf{n}$ is the unit normal

$$\delta\mathbf{g}_N = (\boldsymbol{\eta}^2 - \boldsymbol{\eta}^1) \cdot \mathbf{n} \quad (2.22)$$

$$\Pi(\mathbf{u}) = \frac{1}{2} \mathbf{u}^T \mathbf{K} \mathbf{u} - \mathbf{u}^T \bar{\mathbf{f}} + \lambda \mathbf{G}^T \mathbf{u} \quad (2.23)$$

$$\text{And } \mathbf{g} = \mathbf{G}^T \mathbf{u} \quad (2.24)$$

$$\text{For } \boldsymbol{\eta} = \delta\mathbf{u}, \quad (2.25)$$

$$\begin{bmatrix} \mathbf{K} & \mathbf{G} \\ \mathbf{G}^T & \mathbf{0} \end{bmatrix} \begin{Bmatrix} \mathbf{u} \\ \lambda \end{Bmatrix} = \begin{bmatrix} \mathbf{f} \\ \mathbf{g} \end{bmatrix} \quad (2.26)$$

The contact contribution to the global stiffness matrix in Lagrange's multiplier formulation is explained by adapting form (Wriggers, p.164-166).

2.3.2 Analytically shell modeling

The internal strain energy in (2.15) can be expressed by two parts ;

$$U = U_b + U_s \quad (2.27)$$

The bending strain energy is;

$$U_b = \frac{1}{2} \int_{\Omega} \mathbf{\epsilon}^T \mathbf{\epsilon}_b d\Omega \quad (2.28)$$

And the transverse shear strain energy is;

$$U_s = \sum_e \frac{1}{2} \int_{\Omega^e} \mathbf{\epsilon}^T \mathbf{\epsilon}_s d\Omega \quad (2.29)$$

where superscript a “e” is indicating “element”

Kinematic matrices $\mathbf{B}_b$ and $\mathbf{B}_s$ are;

$$[\mathbf{B}_b] = [[\mathbf{B}_{b1}] \quad [\mathbf{B}_{b2}] \quad [\mathbf{B}_{b3}] \quad [\mathbf{B}_{b4}]] \quad (2.30)$$

In terms of shape functions;

$$[\mathbf{B}_{bi}] = \begin{bmatrix} H_1 \frac{\partial N_i}{\partial x} & 0 & H_2 \frac{\partial N_i}{\partial x} & 0 & 0 \\ 0 & H_1 \frac{\partial N_i}{\partial y} & 0 & H_2 \frac{\partial N_i}{\partial y} & 0 \\ H_1 \frac{\partial N_i}{\partial y} & H_1 \frac{\partial N_i}{\partial x} & H_2 \frac{\partial N_i}{\partial y} & H_2 \frac{\partial N_i}{\partial x} & 0 \end{bmatrix} \quad (2.31)$$

$$\text{And} \quad [\mathbf{B}_s] = [[\mathbf{B}_{s1}] \quad [\mathbf{B}_{s2}] \quad [\mathbf{B}_{s3}] \quad [\mathbf{B}_{s4}]] \quad (2.32)$$

$$[\mathbf{B}_{si}] = \begin{bmatrix} N_i \frac{\partial H_1}{\partial z} & 0 & N_i \frac{\partial H_2}{\partial z} & 0 & \frac{\partial N_i}{\partial x} \\ 0 & N_i \frac{\partial H_1}{\partial z} & 0 & N_i \frac{\partial H_2}{\partial z} & \frac{\partial N_i}{\partial y} \end{bmatrix} \quad (2.33)$$

The element stiffness matrix can be expressed as;

$$[\mathbf{K}^e] = \int_{\Omega^e} [\mathbf{B}_b]^T [\mathbf{D}_b] [\mathbf{B}_b] d\Omega + \int_{\Omega^e} [\mathbf{B}_s]^T [\mathbf{D}_s] [\mathbf{B}_s] d\Omega \quad (2.34)$$

The plate bending element where x, y and z describe the global coordinates of the plate and u, v and w are the displacements and ξ , η , ζ are local coordinates. The x-y

plane is parallel to the midplane prior to deflection. Using isoparametric elements the three displacements can be expressed as;

$$\mathbf{u} = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} N_i(\xi, \eta) H_j(\zeta) \mathbf{u}_{ij} \quad (2.35)$$

$$\mathbf{v} = \sum_{i=1}^{N_1} \sum_{j=1}^{N_2} N_i(\xi, \eta) H_j(\zeta) \mathbf{v}_{ij} \quad (2.36)$$

$$\mathbf{w} = \sum_{i=1}^{N_1} N_i(\xi, \eta) \mathbf{w}_i \quad (2.37)$$

The bending and transverse shear strains as a function of displacement are;

$$\boldsymbol{\epsilon}_b = \begin{Bmatrix} \epsilon_x \\ \epsilon_y \\ \gamma_{xy} \end{Bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & 0 \\ 0 & \frac{\partial}{\partial y} & 0 \\ \frac{\partial}{\partial y} & \frac{\partial}{\partial x} & 0 \end{bmatrix} \begin{Bmatrix} u \\ v \\ w \end{Bmatrix} \quad (2.38)$$

$$\boldsymbol{\epsilon}_s = \begin{Bmatrix} \gamma_{yz} \\ \gamma_{xz} \end{Bmatrix} = \begin{bmatrix} \frac{\partial}{\partial x} & 0 & \frac{\partial}{\partial x} \\ 0 & \frac{\partial}{\partial z} & \frac{\partial}{\partial y} \end{bmatrix} \begin{Bmatrix} u \\ v \\ w \end{Bmatrix} \quad (2.39)$$

Bending and shear strains in terms of kinematic matrices;

$$\boldsymbol{\epsilon}_b = \mathbf{B}_b \mathbf{d} \quad (2.40)$$

$$\boldsymbol{\epsilon}_s = \mathbf{B}_s \mathbf{d} \quad (2.41)$$

The constitutive equations for bending and shear;

$$\boldsymbol{\sigma}_b = \mathbf{D}_b \boldsymbol{\epsilon}_b \quad (2.42)$$

$$\boldsymbol{\sigma}_s = \mathbf{D}_s \boldsymbol{\epsilon}_s \quad (2.43)$$

$$\boldsymbol{\sigma}_s = \boldsymbol{\tau}_{yz} \quad (2.44)$$

The material property matrices for the plane stress conditions, for an unidirectional composite material is;

$$[D_b] = \begin{bmatrix} D_{11} & D_{12} & 0 \\ D_{12} & D_{22} & 0 \\ 0 & 0 & D_{33} \end{bmatrix} \quad (2.45)$$

$$\mathbf{p}_s = \frac{E}{2(1+\nu)} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \quad (2.46)$$

E_{ij} is the elastic modulus, G_{ij} is the shear modulus and ν_{ij} is the poisson ratio. Where the components in transverse and longitudinal directions are;

$$D_{11} = \frac{E_1}{1 - \nu_{12}\nu_{21}} \quad (2.47)$$

$$D_{12} = \frac{E_1\nu_{21}}{1 - \nu_{12}\nu_{21}} \quad (2.48)$$

$$D_{13} = G_{12} \quad (2.49)$$

$$D_s = \begin{bmatrix} G_{13} & 0 \\ 0 & G_{12} \end{bmatrix} \quad (2.50)$$

Firstly, the internal strain energy is expressed by internal strain and transverse shear strain energy. The element stiffness and elastic strains is written in terms of kinematic matrices. Subsequently, constitutive equations are written in terms of material property matrices for unidirectional orthotropic material. The analytical finite element modeling with shell element assumption is explained by adapting from (Kwon & Bang., p.373-377).

3. MODELING OF THE REPRESENTATIVE VOLUME ELEMENT BY USING FINITE ELEMENT METHOD

Finite element modeling of a contact problem requires intense computations. There are two main difficulties. Firstly, searching for possible contact regions and preventing from abrupt contact status changes during simulation. Secondly, friction existing in the contact region makes analysis highly nonlinear (Ansys® Analysis Guide).

Thus finite element modeling and computations are done via Ansys® Academic Research, Release 11.0.

3.1 Contact Problem Type

Contact problems can be classified with two general classes: Rigid-flexible and flexible-flexible. Flexible-flexible type of contact is usually using for deformable bodies which is also the case here. Five contact capabilities are available in Ansys®; node-node, node-surface, surface-surface, line-line. The possible contact pairs recognize via contact elements defined with contact tool. These are; for surface to surface contact; Conta171, Conta 172, Conta 173, Conta174 are in use. For line-line contact, Conta176; for line-surface contact, Conta177; for node-surface, Conta175; for node-node Conta 178, Conta12, Conta52 are in use as contact elements while for node-surface and surface-surface contact Targe169 and for line-line, line-surface and surface-surface Conta 170 is in use (Ansys® Analysis Guide).

There are two options for constructing contact pairs: Symmetric and asymmetric contact pairs. The asymmetric contact is more convenient for surface to surface contact in which contact target and contact elements are definable, having the advantage to require fewer computations.

3.2 Contact Problem Solution Algorithms

Augmented Lagrange, Pure Penalty, MPC, Normal Lagrange are the formulations that Ansys® use for contact problems.

The basic differences between the Penalty and the Lagrange Methods are: The penalty method is based on the assumption of “spring” which connects the two surfaces, called contact stiffness.

$$\mathbf{K}_{contact} \Delta \mathbf{x}_{penetration} = \Delta \mathbf{F}_{contact} \quad (3.1)$$

The Augmented Lagrange method uses an iterative series of penalty methods.

$$[\mathbf{K}]\{\mathbf{x}\} = \{\mathbf{F}\} + \{F_{contact}\} \quad (3.2)$$

Which theoretically gives the possibility of to have zero penetration. For the Augmented Lagrange method, the contact stiffness is updated per contact element by the force (pressure) λ ;

$$\lambda_{i+1} = \lambda_i + \mathbf{K}_{contact} \mathbf{x}_{penetration} \quad (3.3)$$

Iterations are continued until penetration within the allowable limits (Ansys® Analysis Guide).

3.3 Computing Performance and Solver Types

Ansys®’s memory is divided into two spaces: Database and scratch space. Database memory is used for the model data, and the scratch space is used by the solvers, temporary calculations, graphics, images...etc. Initial memory settings are: Total workspace: 5000MB, Database: 504MB. The high-performance computing (HPC) is set up to use shared memory parallel (SMP) with 2 processors. Thus, Ansys® uses multiple processors in a single computer using shared memory architecture. This reduces the CPU time significantly (Ansys® Analysis Guide).

3.3.1 PCG solver

It is a type of direct solver. The logic is based on guessing a solution vector and update it every iteration for static analysis

$$[\mathbf{K}]\{\mathbf{u}\} = \{\mathbf{F}\} \quad (3.4)$$

The solution converges after satisfying the condition,

$$\frac{\{R_i\}^T \{R_i\}}{\{F\}^T \{F\}} \leq \varepsilon^2 \quad (3.5)$$

where $\{R_i\}$ is the residual vector and ε is the tolerance value which is default 1e-8 for static analysis.

$$\{R_i\} = \{F\} - [K]\{u_i\} \quad (3.6)$$

The memory managements are less compared to direct solvers and computation time is less but difficult for ill-conditioned cases (Ansys® Analysis Guide).

Direct solvers have advantages to solve nonlinearities; shell elements, supports all materials, elements...etc. But has difficulties in computation because matrix inversion requires intensive memory effort. There are two direct solver types: Frontal (Wavefront) solver and the sparse solver.

3.3.2 Sparse direct solver

Sparse matrix by nature easily compressed and this results significantly less computer data storage use. The linear equation (3.4) can be solved by triangular decomposition of a matrix $[K]$.

$$[L][U]\{u\} = \{F\} \quad (3.7)$$

where $[L]$: lower triangle matrix

$[U]$: upper triangular matrix

By substituting, $\{w\} = [U]\{u\}$ (3.8)

For symmetric $[K]$;

$$K = L^T D L \quad (3.9)$$

where $[D]$ is a diagonal matrix and equation and equation (3.7) and can be expressed via Cholesky decomposition (Ansys® Analysis Guide);

$$L^T D L = \begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{bmatrix} \quad (3.10)$$

$$\begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} a_{11} & 0 & 0 \\ 0 & a_{22} & 0 \\ 0 & 0 & a_{33} \end{bmatrix} \quad (3.11)$$

$$\mathbf{L}^T \mathbf{K} \mathbf{L} \mathbf{U} = \mathbf{F} \quad (3.12)$$

And

$$\mathbf{L}^T \mathbf{L}^T \mathbf{K} \mathbf{L} \mathbf{U} = \mathbf{F} \quad (3.13)$$

3.4 Representative Volume Element Model Parameters

Numerical model parameters generated via Matlab®. The keypoints of the carbon nanotube is created in batch mode, by APDL (Ansys® Parametric Development Language). Keypoints can be seen in Figure 3.1.

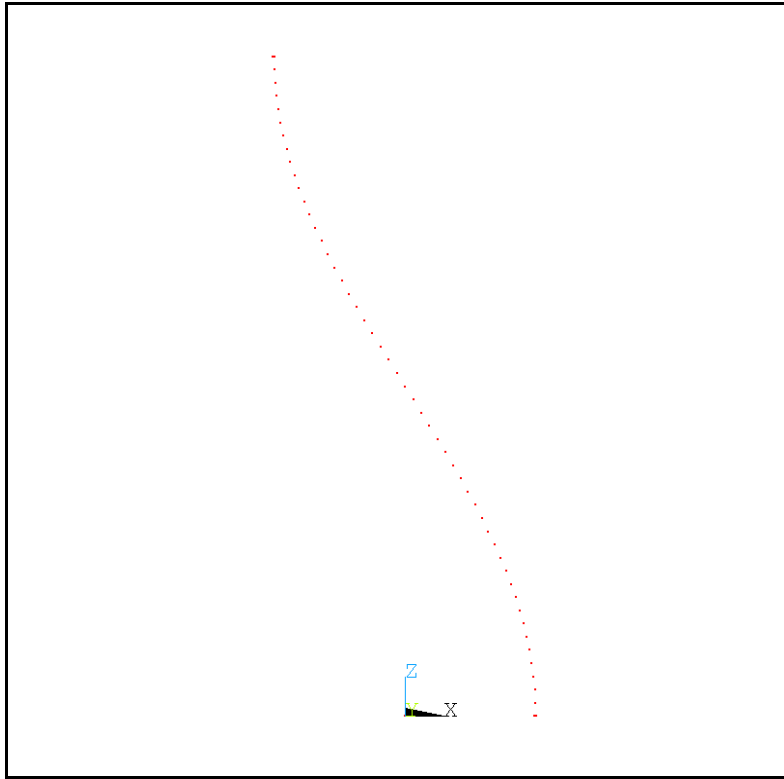


Figure 3.1: Keypoints of curved carbon nanotube

The carbon nanotubes studied have curved shapes and are modeled by sinusoidal geometry consideration as used by (Fisher et al., 2003). The spatial position in the xyz cartesian coordinates is given by

$$z = A \sin \frac{2\pi x}{\lambda} \quad (3.14)$$

Where A is the amplitude of the function and λ is the wavelength. The waviness ratio is A/λ where λ is the length of the nanotube (Fisher et al. 2003).

The waviness ratio used in this study is 0.2 where the wave length is 250 nm and the diameter of carbon nanotube is 2 nm. Furthermore, in this study two models having different waviness ratio (0.2; 0.3) are studied.

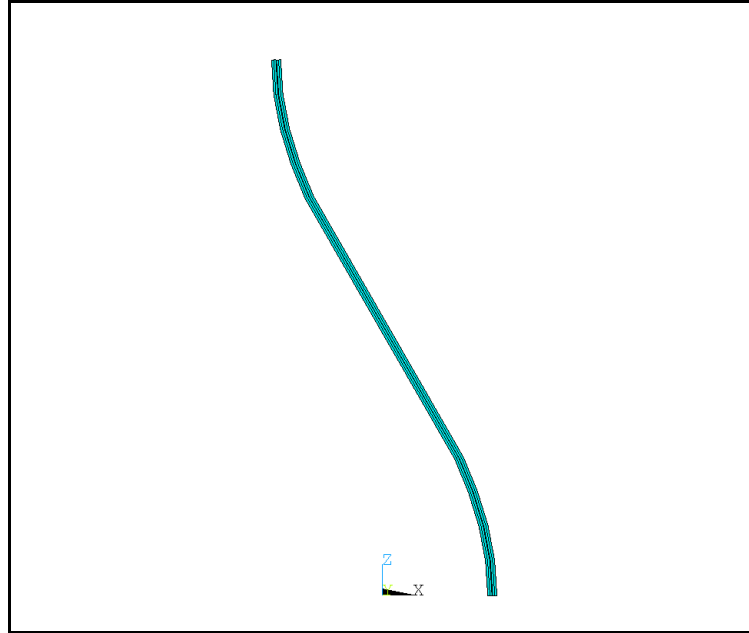


Figure 3.2: Carbon nanotube Shells having 0.34 nm thickness

The carbon nanotube model is created using a spline which connects the keypoints and a circle of a radius 1 nm (Figure 3.2). Volume is created through a circle and a spline which is subtracted from a block of dimensions 400x50x250 nm³ (Figure 3.3 and Figure 3.4). The block is namely, representative volume element and its dimensions are the same for all case studied.

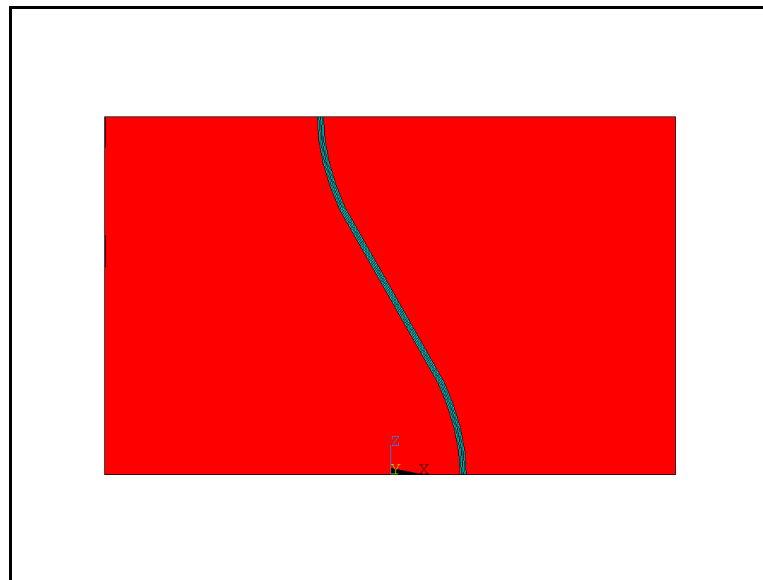


Figure 3.3: Representative Volume Element with Two Aligned Carbon Nanotubes

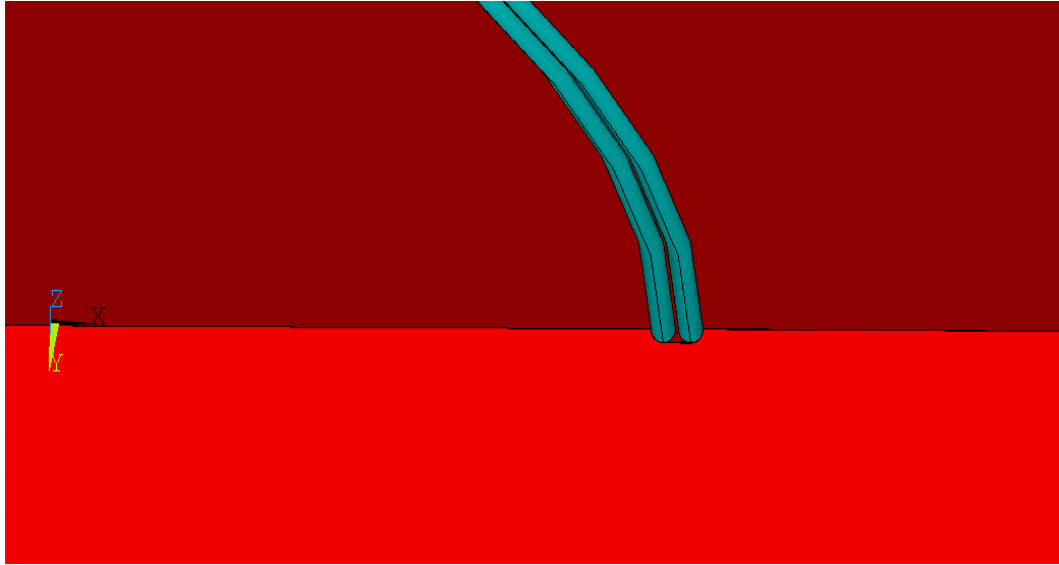


Figure 3.4: Representative Volume Element with Two Aligned Carbon Nanotube (Zoomed View)

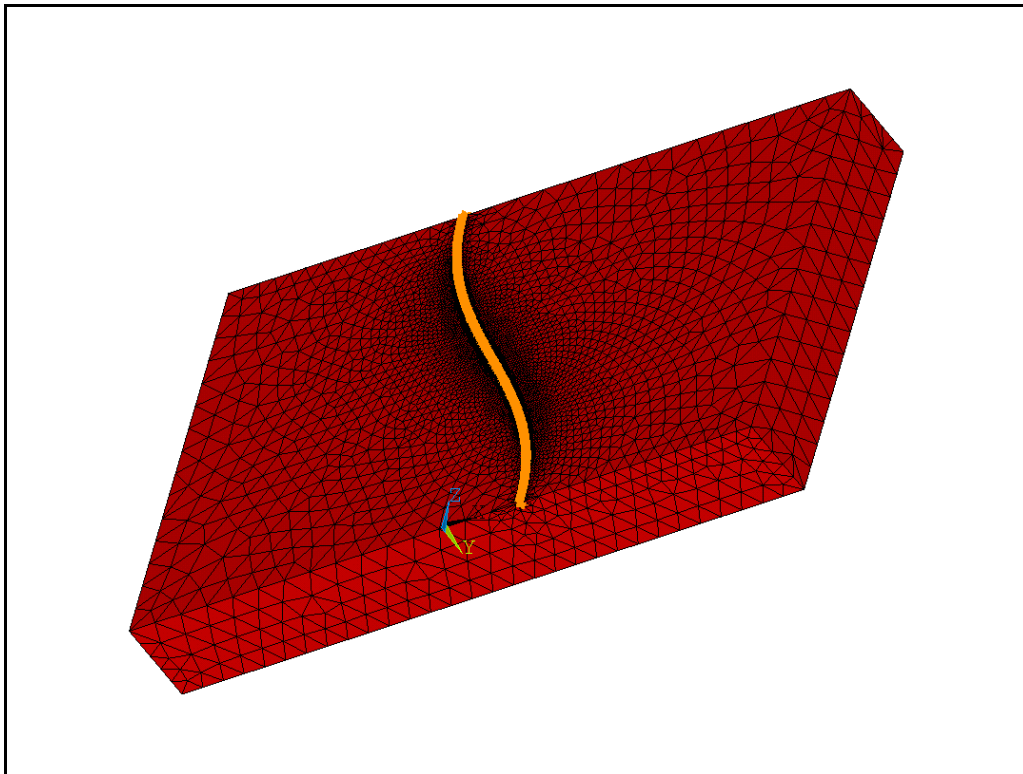


Figure 3.5: The Finite Element Model of the Representative Volume Element

The carbon nanotubes' element type is 8-Node Shell 181 Element and meshes have quad shapes with pyramids having one degree of freedom and midside nodes follow curves (Figure 3.5). Volume element is the 10-Node Tetrahedral Structural Solid 186. The meshes have a triangular shape with pyramids having one degree of freedom and midside nodes follow curves. Carbon nanotubes are considered

isotropic having an elastic modulus $E=1000$ GPa, poisson ratio $\nu=0.3$. Epoxy is isotropic and have an elastic modulus $E=5$ GPa and poisson ratio $\nu=0.3$.

The Areas having shell element are automatically meshed via mesh tool using shell element elastic 4 node 181. Solid elements are structural solid element 20 node 186. Elements have mid-side nodes and thus gives better accuracy results. The model is symmetrical on the $x=0$ and $y=0$ planes and displacement u_z is different between each case. Shell section (Figure 3.6) has a thickness of 0.34 nm and offset location is the top plane.

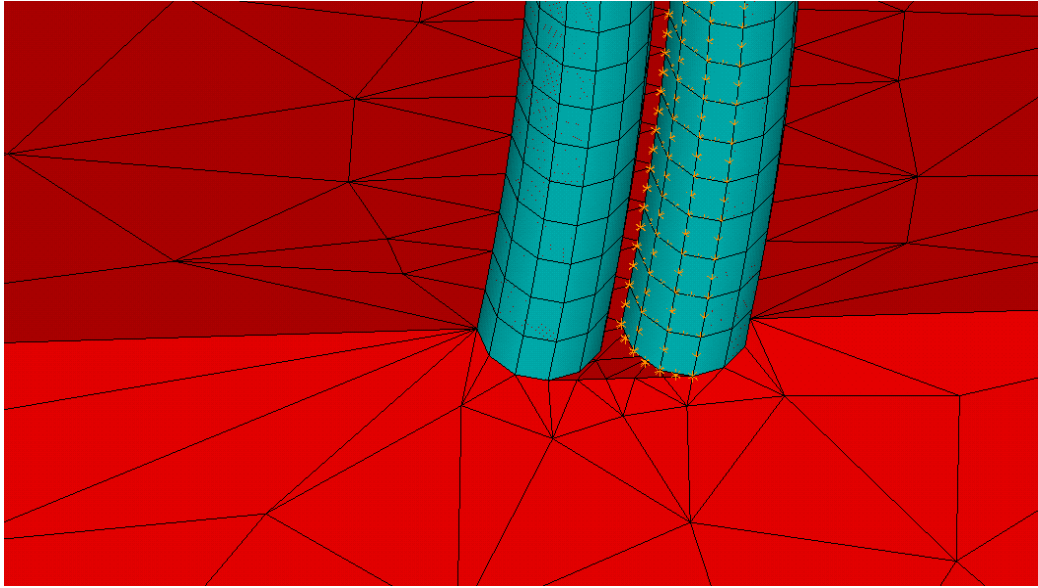


Figure 3.6: The zoomed view of the finite element model of the carbon nanotubes

3.5 Contact Parameters

The contact status defined in Ansys® are: Open far-field contact, open near-field contact, sliding contact, sticking contact. The pinball region is defined from the user is a circle for 2D analysis and sphere for 3D analysis. The contact status definition depends on the position of contact nodal points or integration points of contact elements. There are must be within the pinball region for contact condition.

Sticking contact uses the Coulomb friction model which is an equivalent shear stress τ ,

$$\tau = \mu p + COHE \quad (3.15)$$

Where μ is the friction coefficient, the contact pressure p , and COHE is the cohesion in other words, sliding resistance. Sliding contact occurs when the external force is larger than frictional forces, the two surfaces.

The contact surface defined by Ansys® are: Standard unilateral contact, rough frictional contact, no separation contact, bonded contact, no separation contact, fully bonded contact, initially bonded contact. Time step control predicts the contact status variations (Ansys® Analysis Guide).

Contact modeling is performed using contact pair tool. Contact pair is asymmetric, surface to surface and flexible-flexible. Contact is defined with elements Conta 175 and Targe 170. The asymmetric contact is preferred because it reduces CPU time. Rough frictional contact with friction coefficient 0.1 defined because rough friction prevents sliding between contacting bodies. The model is only constrained with symmetric boundary conditions and sliding is not desired. Additionally, between the carbon nanotubes surfaces there are Van der Waals or chemical bonds which didn't modeled molecularly in this thesis. Rough frictional model is considered be an approximation to this phenomenon.

Augmented Lagrange algorithm explained in details in Chapter 2.3.1 is performed. Augmented Lagrange formulation, penetration limits are definable which is more practical in this model. Automatic bisections are used because abrupt contact status changes could be occurred in the model.

Contact detection is defined on Gauss points. In order to augment integration points, 4-node shell 181 element is used with full integration. Shell section have 0° orientation. Analysis is static and nonlinear due to contact model. The analysis is solved in two sub-steps in order to facilitate iteration process. Sparse direct solver, which is based on direct elimination method, is more suitable for models having a defined contact, are used. Models in which contact is defined are solved with the iterative solver, PCG (Preconditioned Conjugate Gradient Method) solver. The default PCG tolerance value 10^8 is set to 10^5 in order to reduce CPU time.

4. NUMERICAL RESULTS

This chapter includes numerical results obtained via Ansys® 11.0. The problem is studied in many cases. The all cases studied are entitled by an abbreviation methodology which is described.

All two cases studied for waviness ratio of 0.2 which is expressed as Case I and a waviness ratio of 0.3 which is expressed as Case II.

For the Case I.1 carbon nanotubes are initially in contact. The model is subjecting the same value of displacement 20 nm in compression. However, the Case 1.2 is a model which carbon nanotubes are come into contact while subjecting a sufficient (different for all sub-cases) displacement value.

The same abbreviation method is used for Case II. Case II.1 is studied with initial contact. It is subjecting the same value of displacement 20 nm in compression for all sub-cases studied. Case II.2 is a model which carbon nanotubes are come into contact while subjecting a sufficient (different for all sub-cases) displacement value.

There are two other cases which are represented by "x" and "y". In the Case "x", representative volume element is not modeled and only carbon nanotubes are analysed. The Case "x" is studied for only Case I.1 and Case II.1. The Case "y" is a model in which the whole model (representative volume element with carbon nanotubes) is subjected displacement in tension. The Case "y" is studied for Case I.2 and Case II.2.

4.1 Case I

The first case includes the geometric data in Table 4.1. Carbon nanotube have a waviness ratio of 0.2 and an aspect ratio of 0.008. Representative volume element aspect ratio is 0.64.

Table 4.1: Geometric data for model

Parameters	Values
Carbon nanotube aspect ratio	0.008
Carbon nanotube waviness ratio	0.2
Representative Volume Element Aspect Ratio	0.64

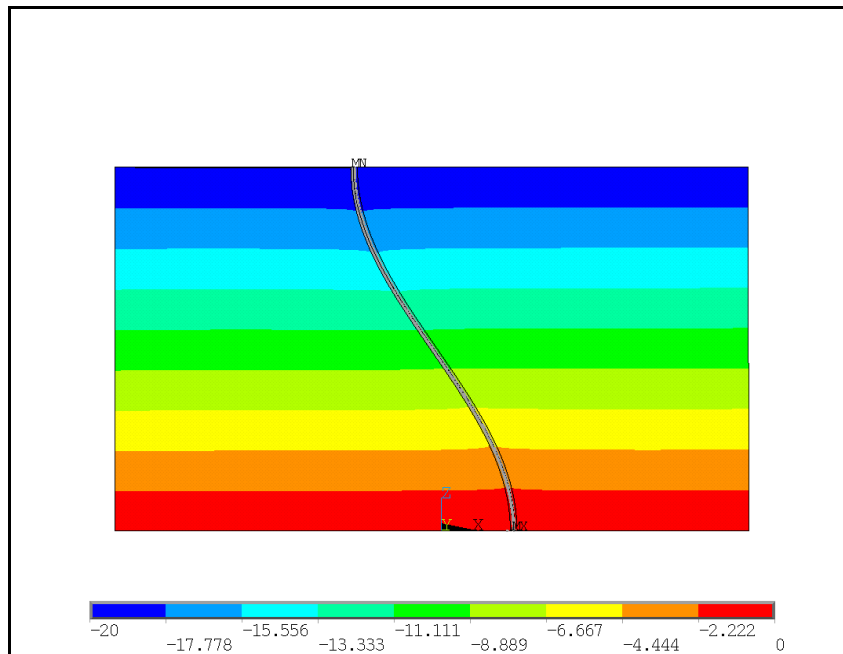
4.1.1 Case I.1

The boundary conditions of the model is given in Table 4.2. The model is symmetric, carbon nanotubes are initially in contact. The model is subjected to 20 nm displacement in compression.

Table 4.2: Boundary Conditions of the Case I.1

Parameters	Values
$U_z(0)$	symmetric
$U_z(250)$	-20 nm
$U_y(0)$	symmetric

Displacement of -20 nm for Case I.1 can be seen in Figure 4.1.

**Figure 4.1:** Displacement values in z direction

Von Mises Equivalent Stress Values (GPa) have maximal and minimal values in the middle of the model as can be seen in Figure 4.2. and in larger extent in Figure 4.3.

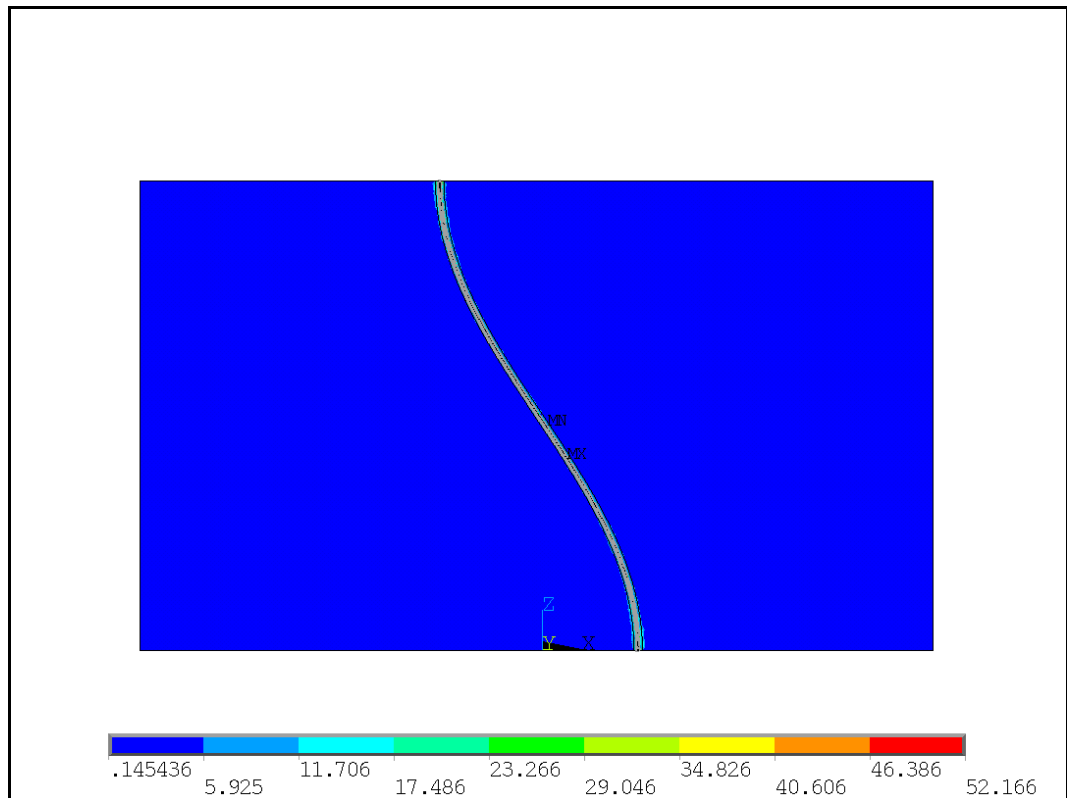


Figure 4.2: Von Mises equivalent Stress Values

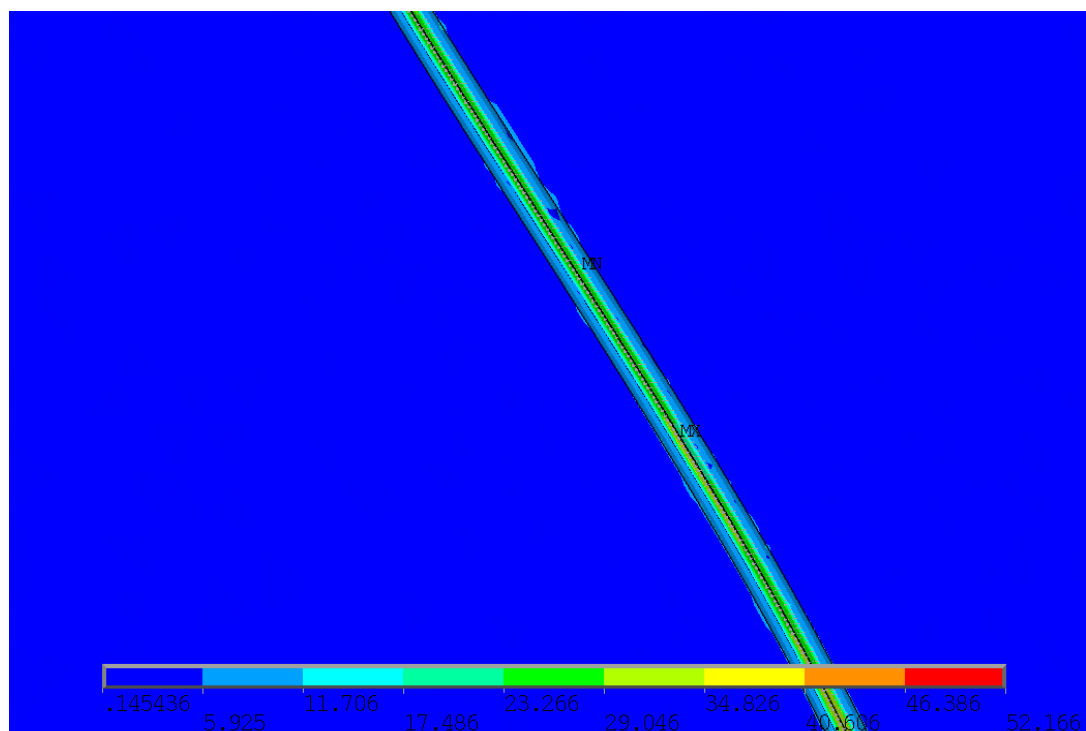


Figure 4.3: Von Mises equivalent Stress Values (Zoomed View)

Von Mises Equivalent Strain (%) have a maximal and minimal value on the top of the model as can be seen in Figure 4.4 and in the larger extent in Figure 4.5.

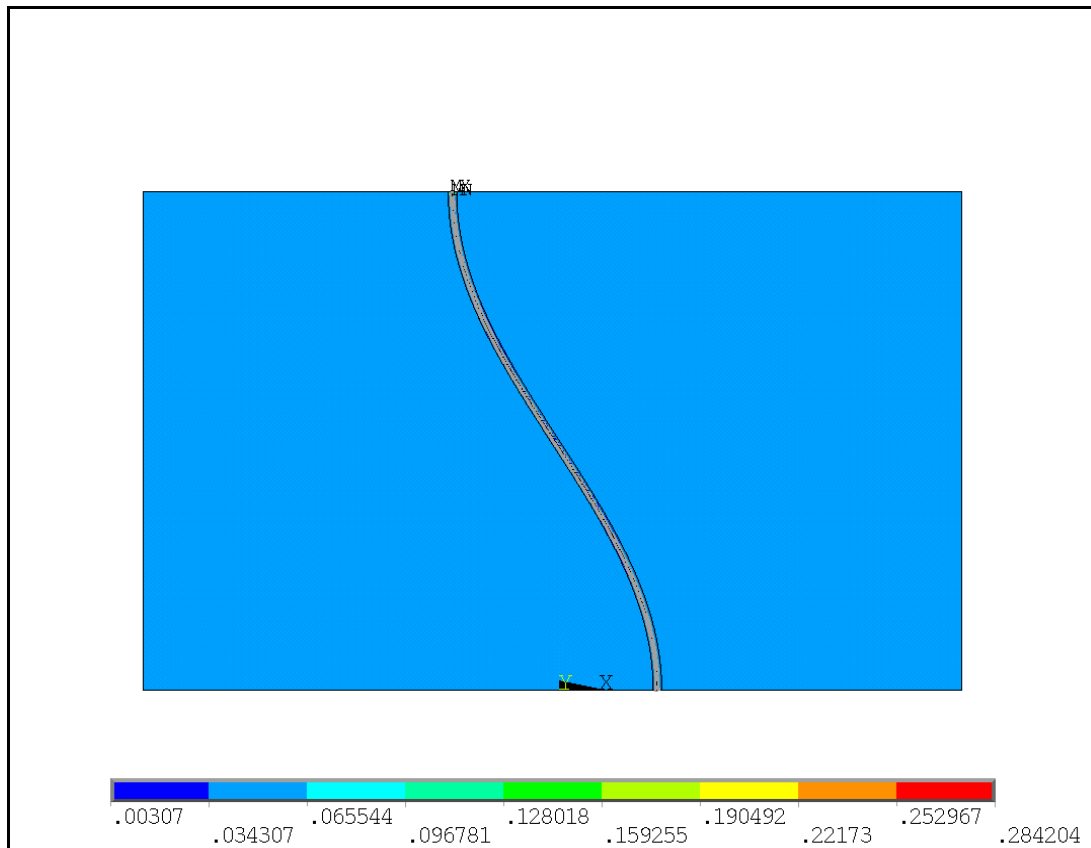


Figure 4.4 : Von Mises Equivalent Elastic Strain

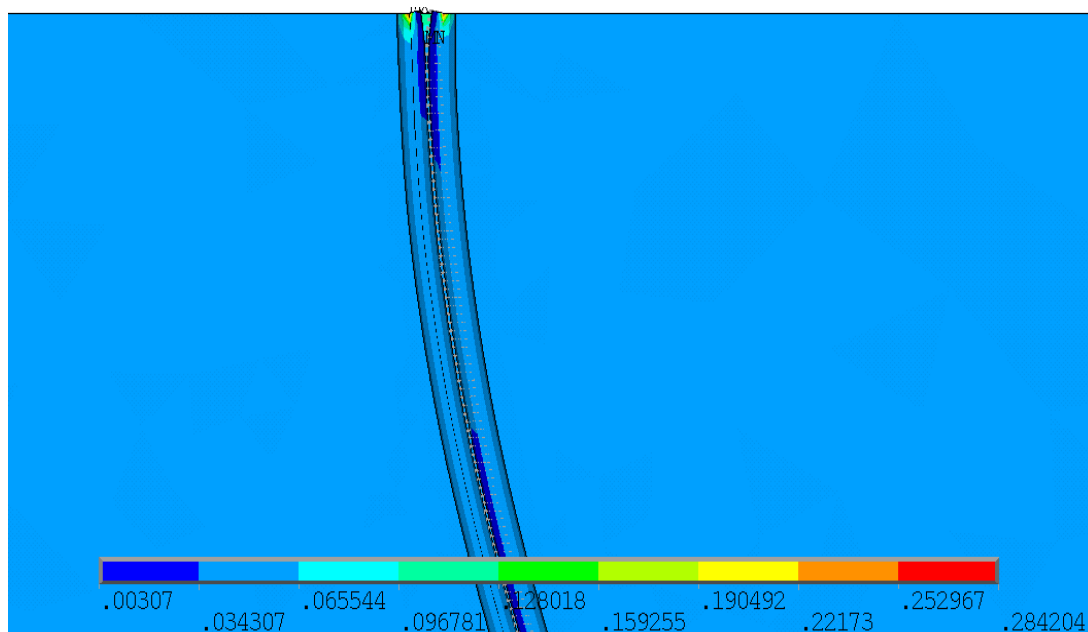


Figure 4.5: Von Mises Equivalent Elastic Strain (Zoomed View)

Contact status is changing from far-open to near-contact, and sticking to sliding. In the middle of the model where the stresses are greater the contact status sticking status can be seen in Figure 4.6 and in larger extent in Figure 4.7.

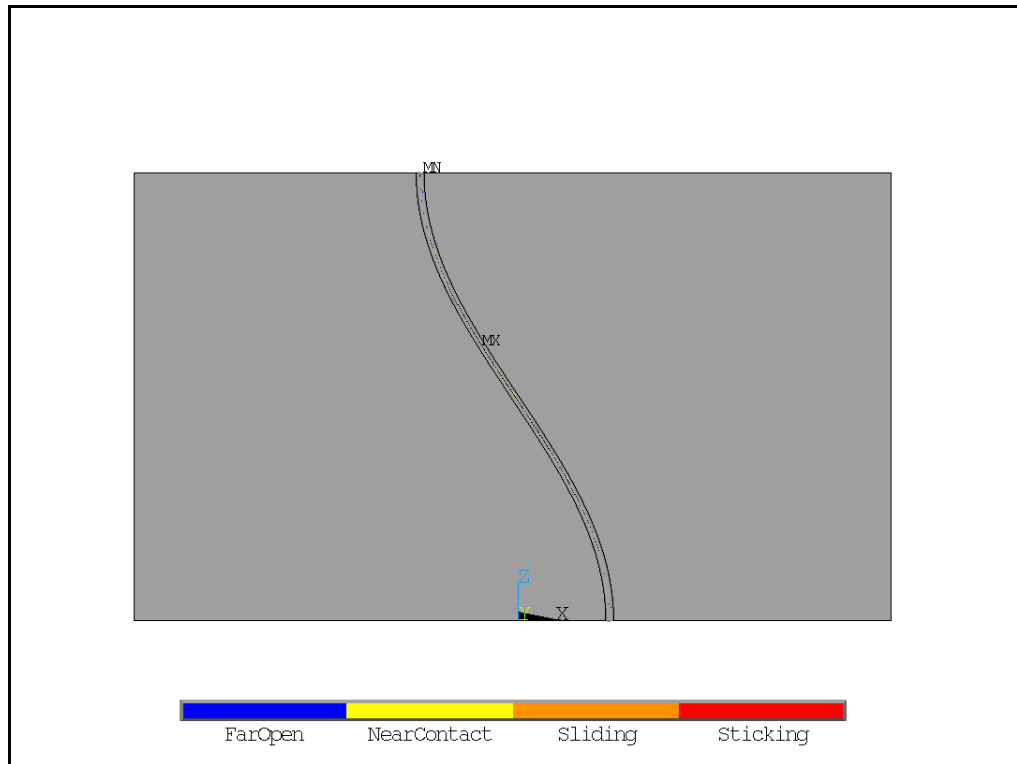


Figure 4.6: Contact Status

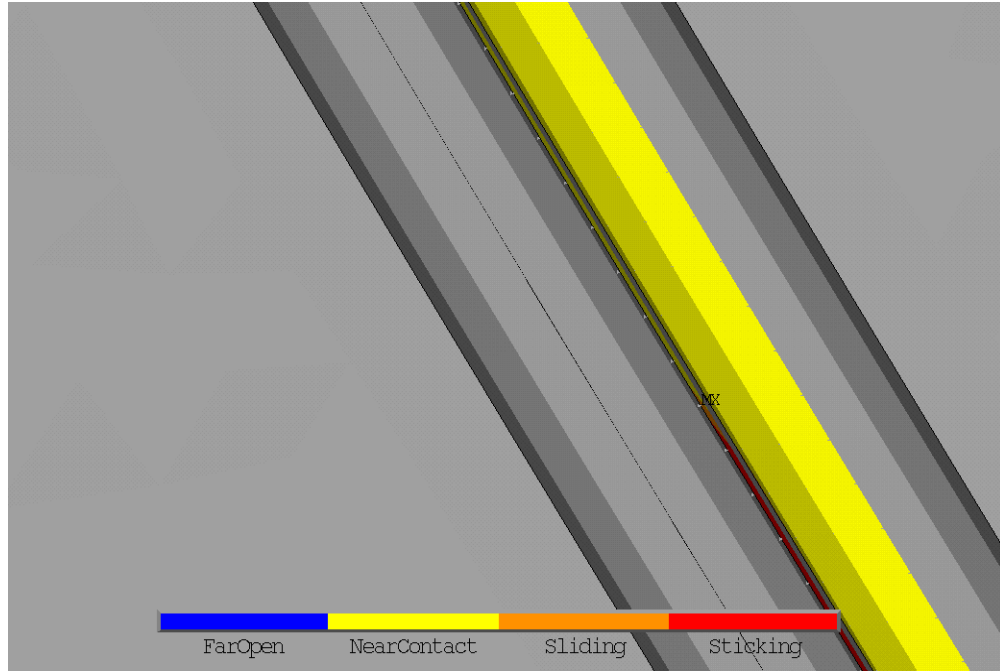


Figure 4.7: Contact Status (Zoomed View)

The numerical results of contact status is shown from Figure 4.6 to Figure 4.7. Contact status is changing from sticking to far-field contact.

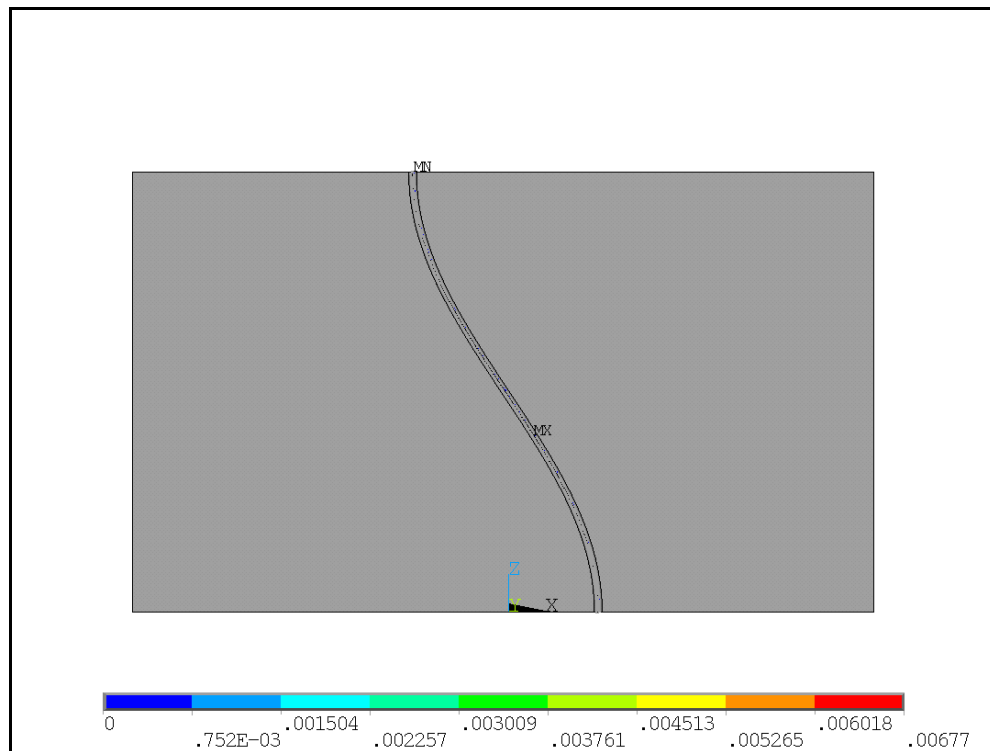


Figure 4.8: Contact Penetration

The contact penetrations' values are 0-0.00677 nm as can be seen in in Figure 4.8 and in Figure 4.9. There not any excessive penetration, the values seems within the allowable limits as defined in the model.

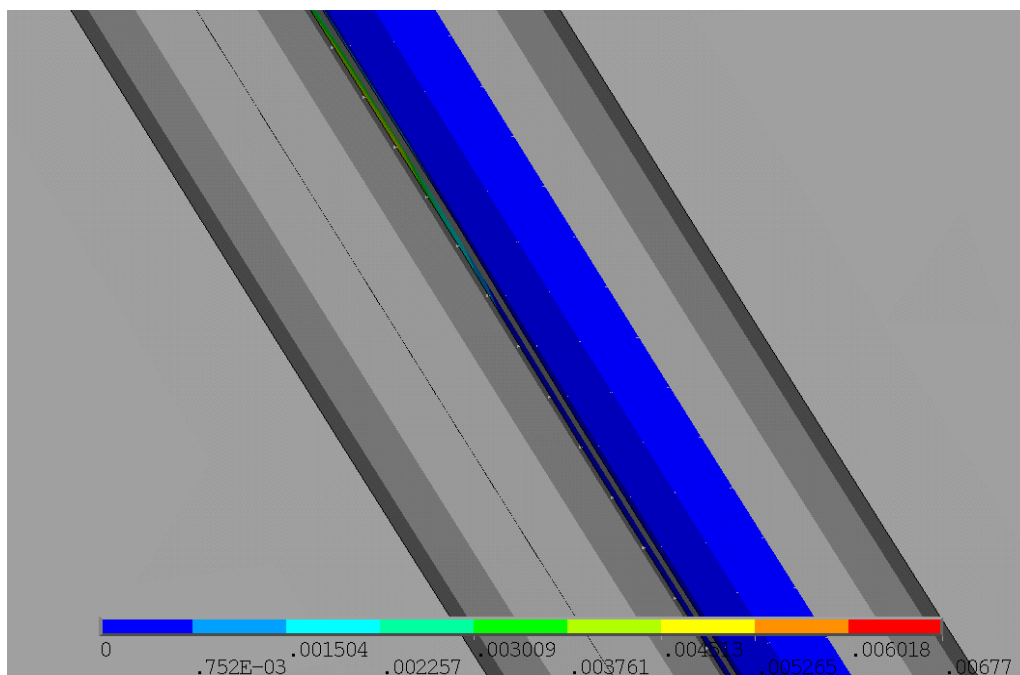


Figure 4.9: Contact Penetration (Zoomed View)

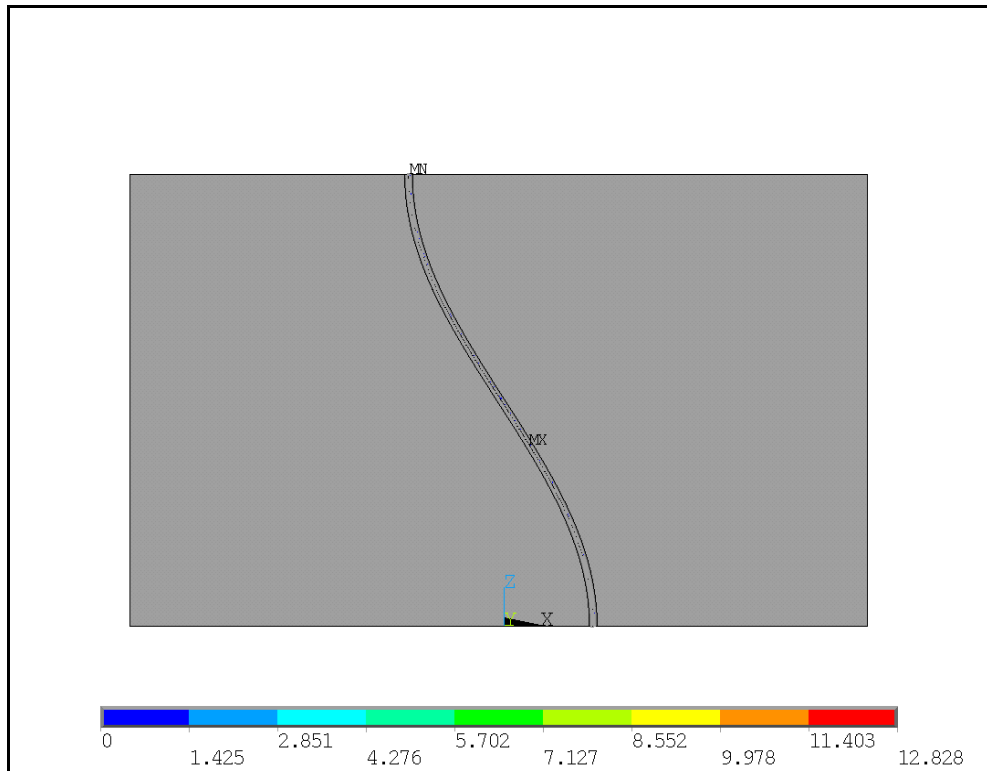


Figure 4.10: Contact Pressure

Contact pressure values are 0-12.828 GPa as can be seen in Figure 4.10 and Figure 4.11.

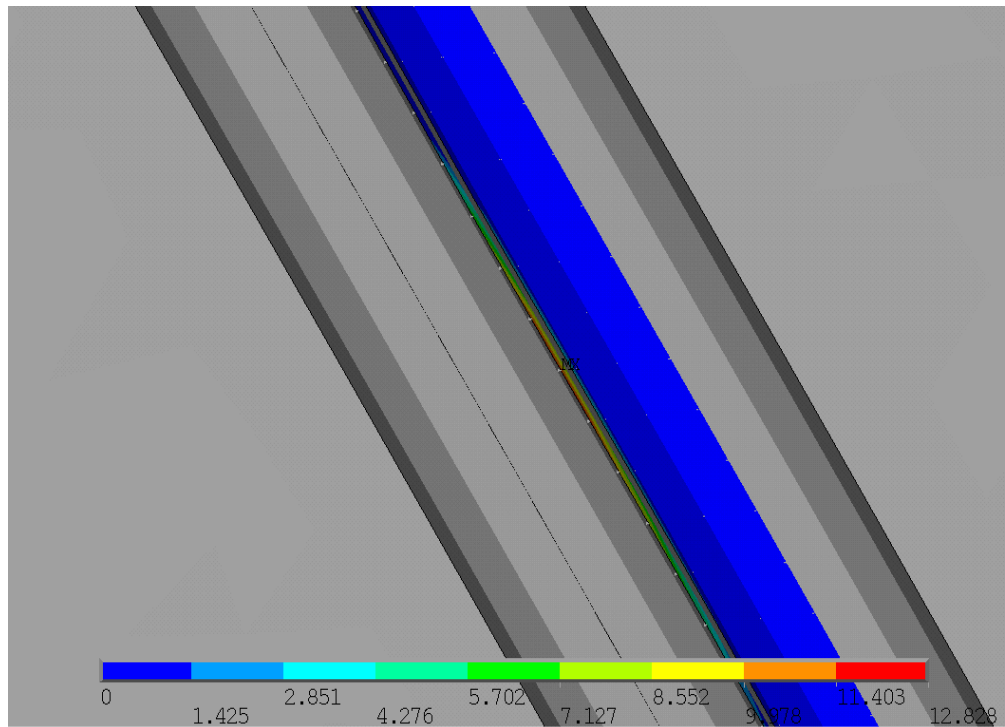


Figure 4.11: Contact Pressure (Zoomed View)

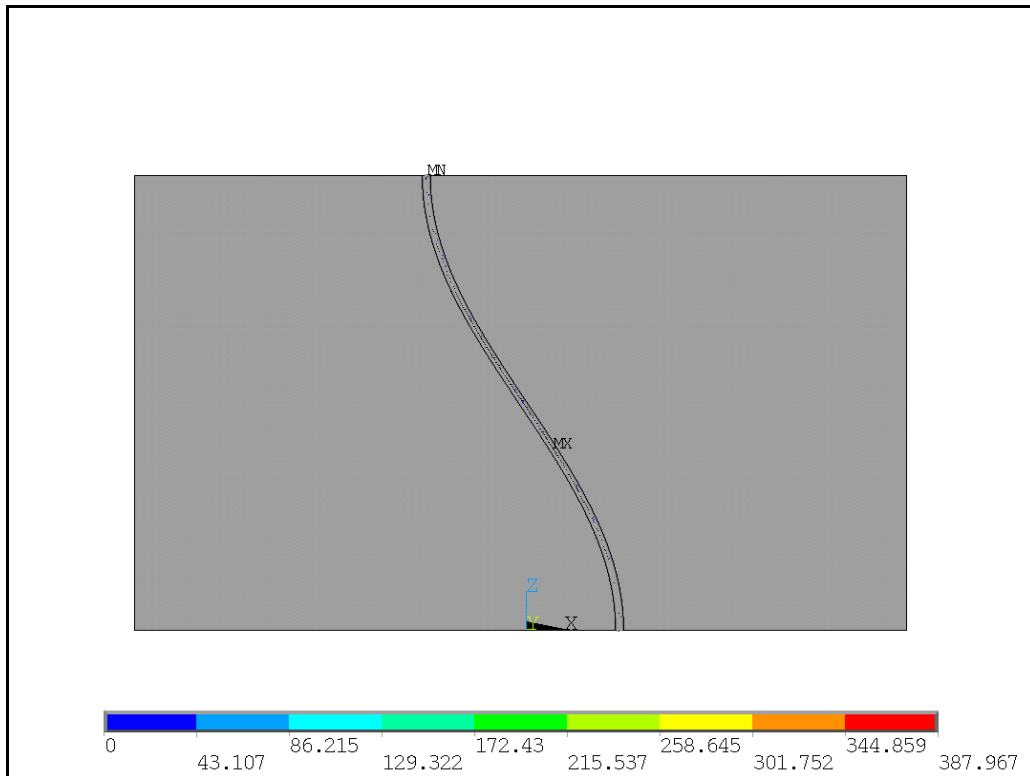


Figure 4.12: Contact Friction Stress

The contact friction stress have values 0-387.967 GPa as can be seen in Figure 4.12 and Figure 4.13.

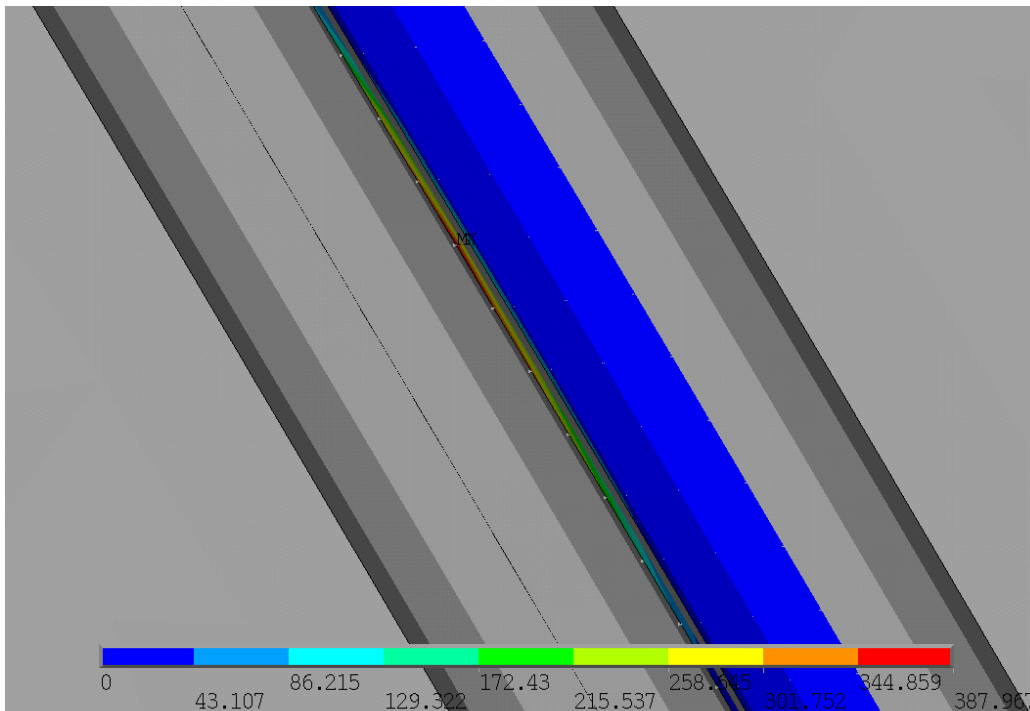


Figure 4.13: Contact Friction Stress (ZoomedView)

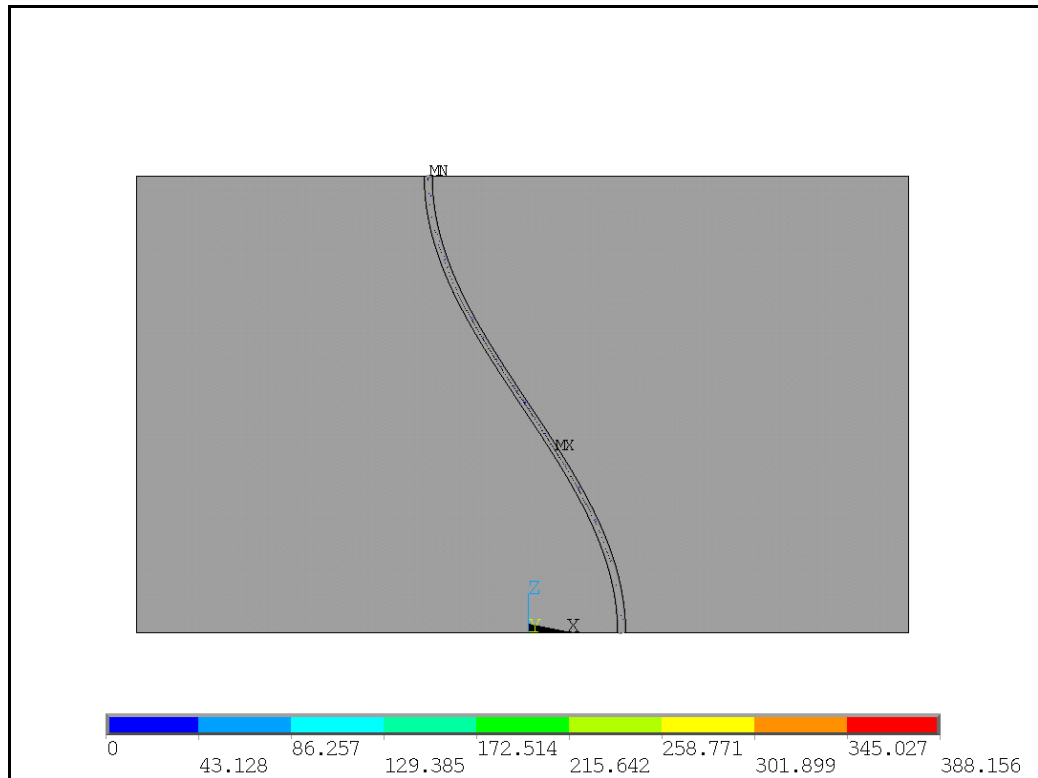


Figure 4.14: Contact Total Stress

Contact total stress have value of 0-388.156 GPa as can be seen in Figure 4.14 and Figure 4.15.

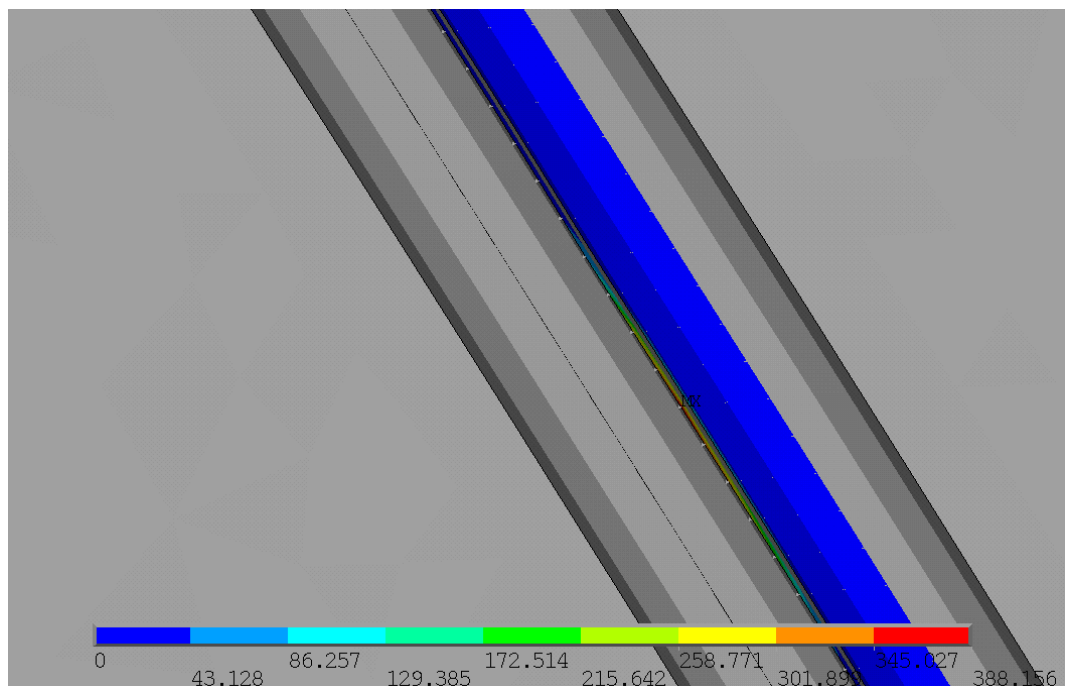


Figure 4.15: Contact Total Stress (Zoomed View)

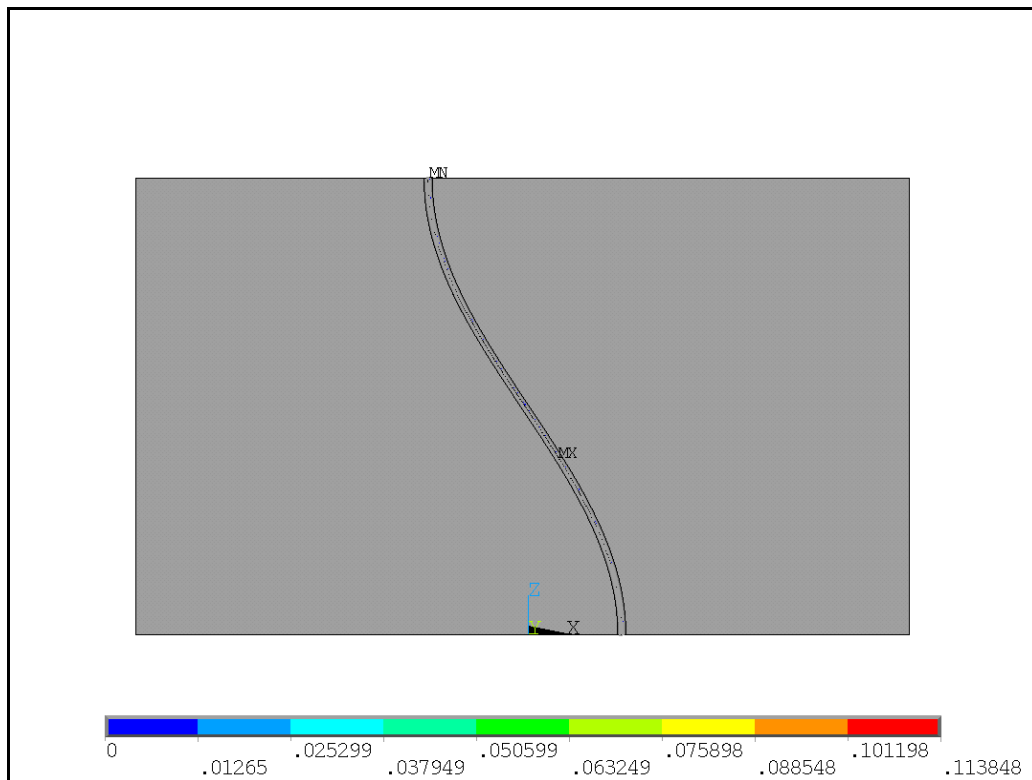


Figure 4.16: Contact Sliding Distance

Contact sliding distance values are 0-0.101198 nm as can be seen in Figure 4.16 and Figure 4.17. The values are within the allowable limits.

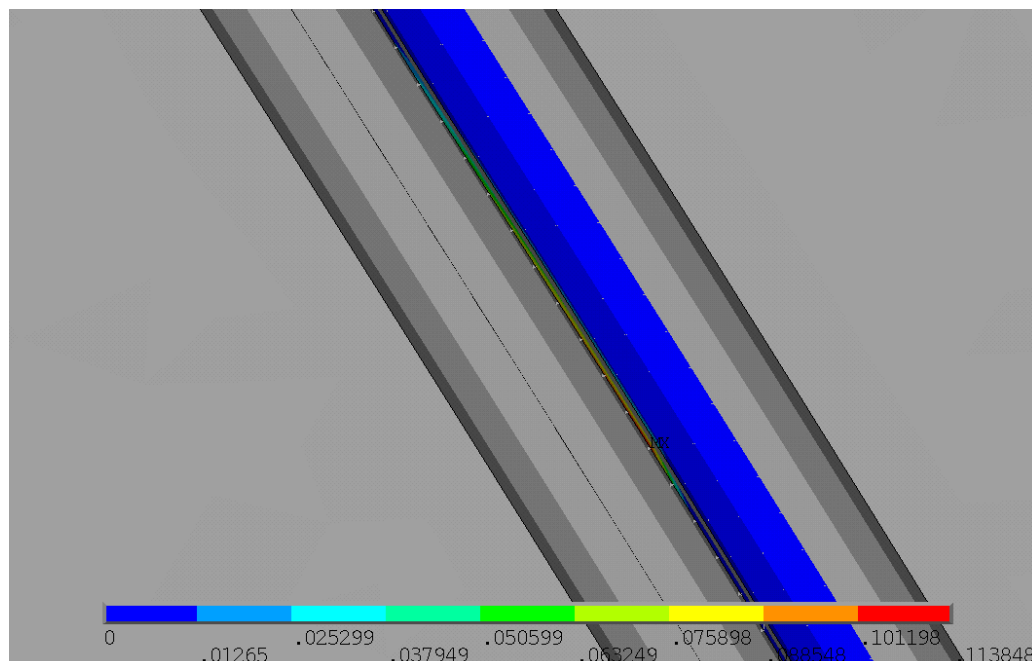


Figure 4.17: Contact Sliding Distance (Zoomed View)

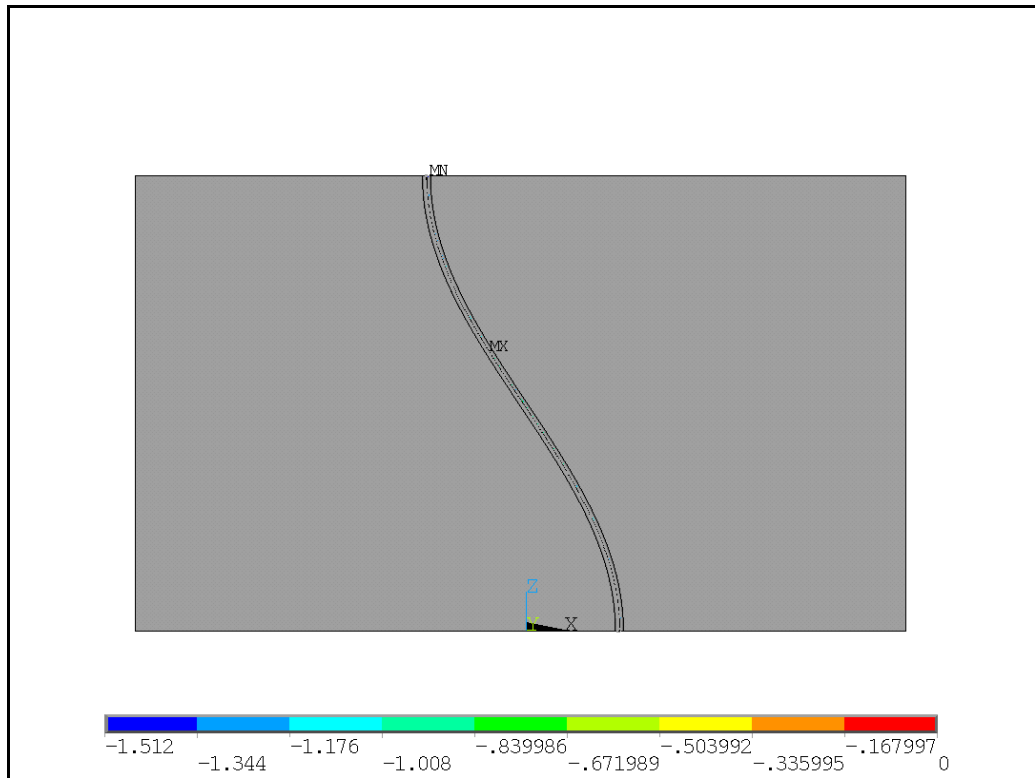


Figure 4.18: Contact Gap Distance

Contact gap distances can be seen in Figure 4.18 and Figure 4.19, are within the allowable penetration values defined. There are not any excessive penetration.

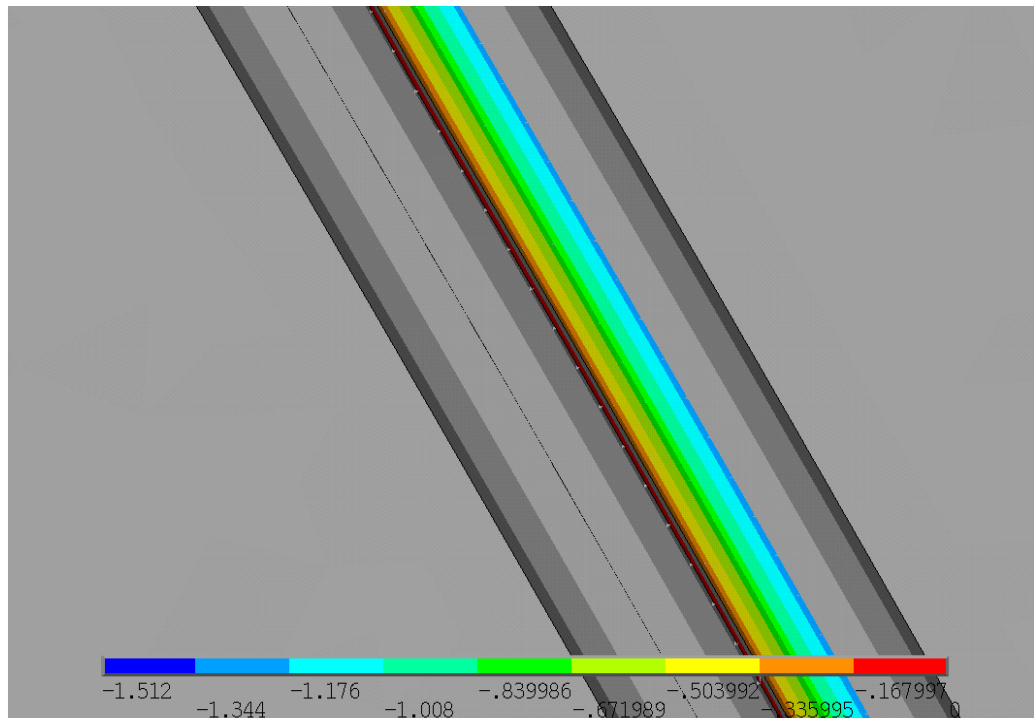


Figure 4.19: Contact Gap Distance (Zoomed View)

4.1.2 Case I.1.x

In this case, the model Case I.1.x is modeled with only carbon nanotubes which are initially in contact. Boundary conditions are the same as in the Table 4.2. The displacement in compression with a 20 nm can be seen in Figure 4.20.

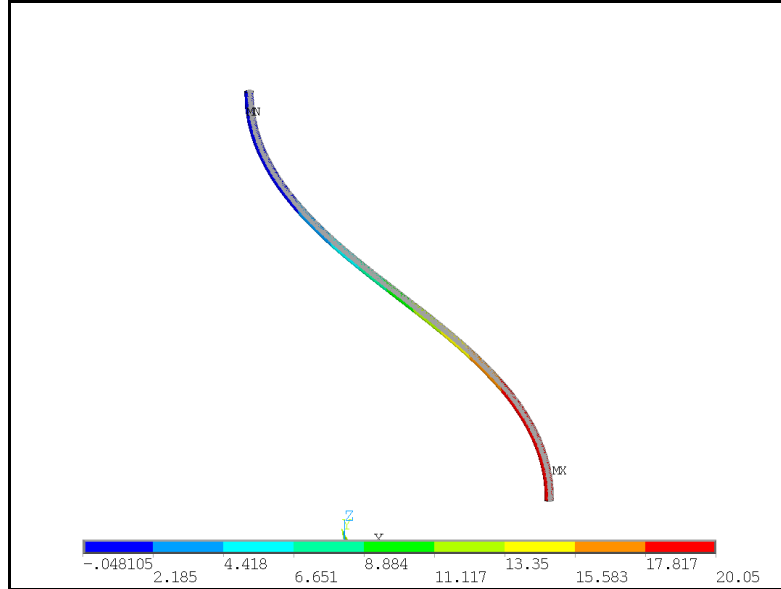


Figure 4.20: Displacement values in z direction

The equivalent Von Mises elastic stress and strains can be seen in Figure 4.21 and Figure 4.22 where two carbon nanotubes are interacting each other. Contact results can be seen from Figure 4.23 to Figure 4.29 where one carbon nanotube is the target surface and the other one is the contact surface.

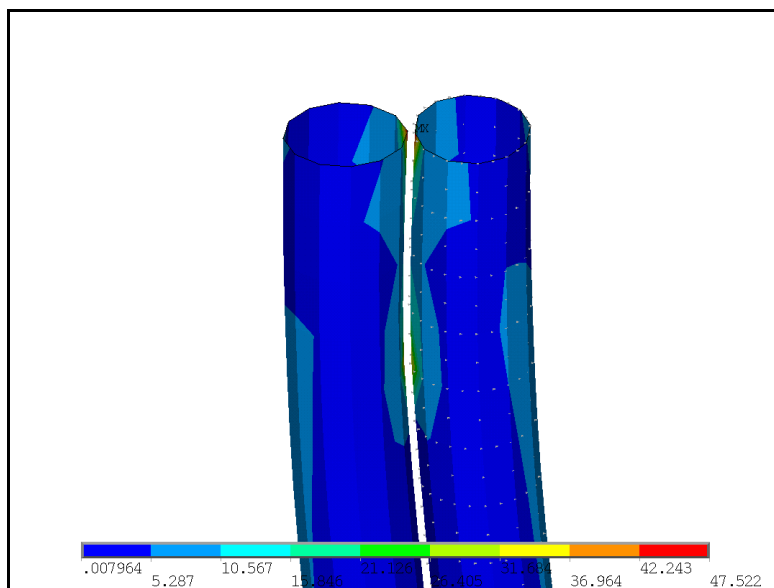


Figure 4.21: Equivalent Von Mises Elastic Stress

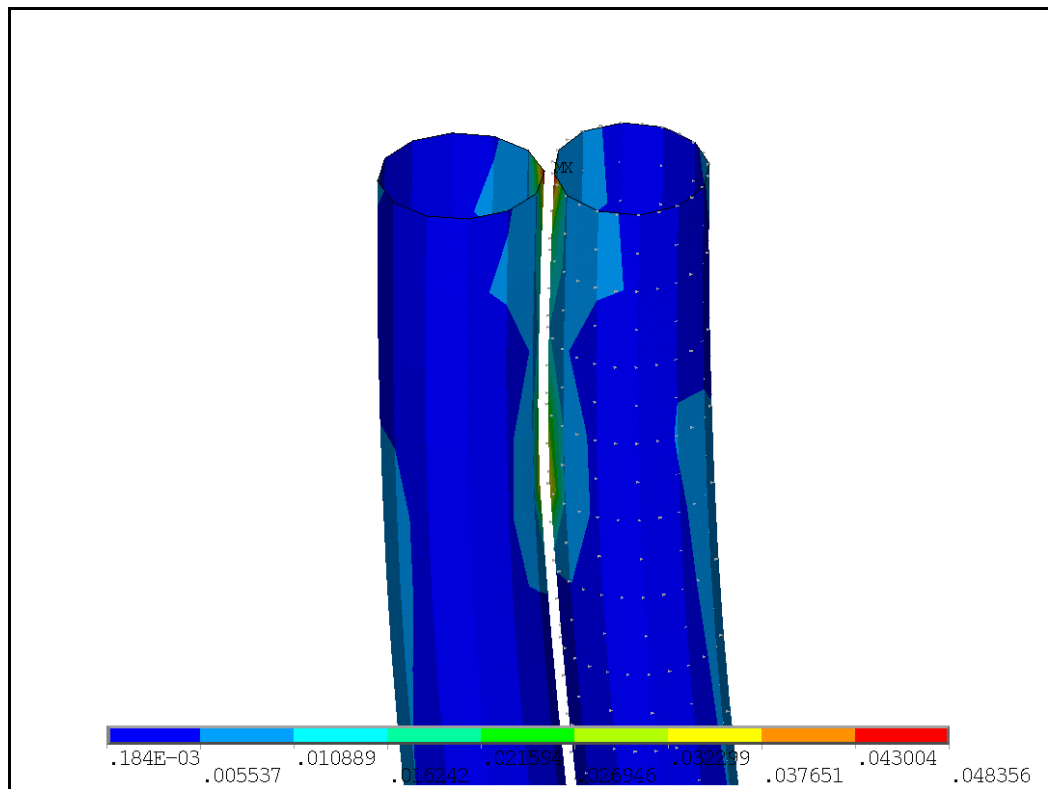


Figure 4.22: Equivalent Von Mises Elastic Strain

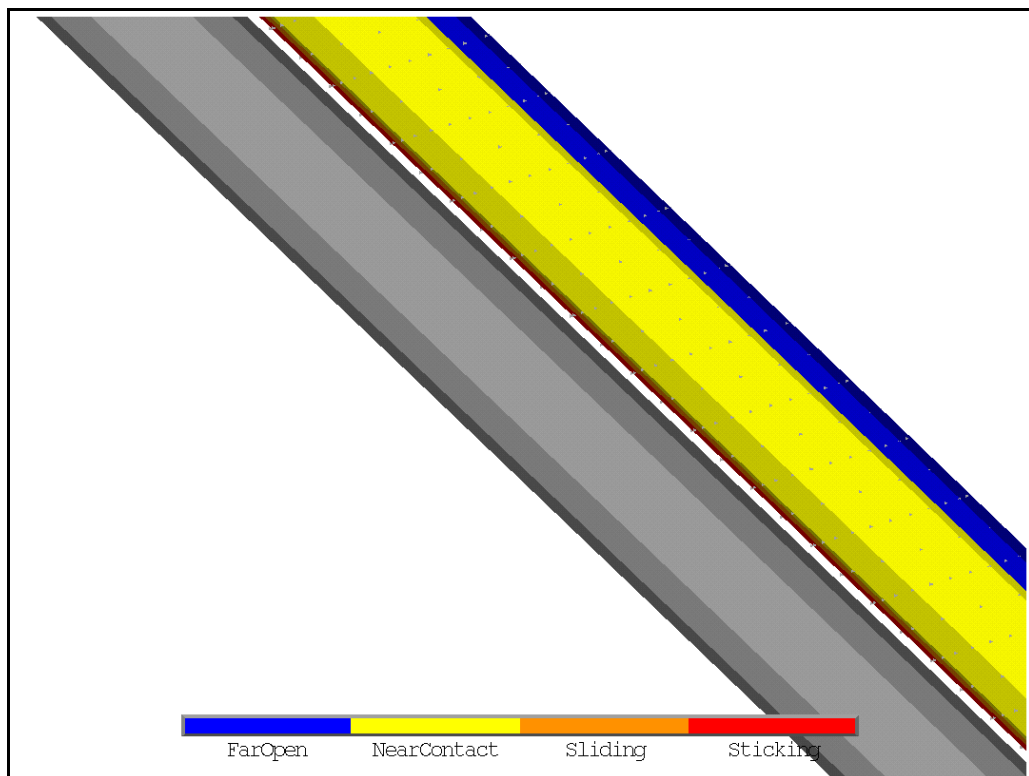


Figure 4.23: Contact Status

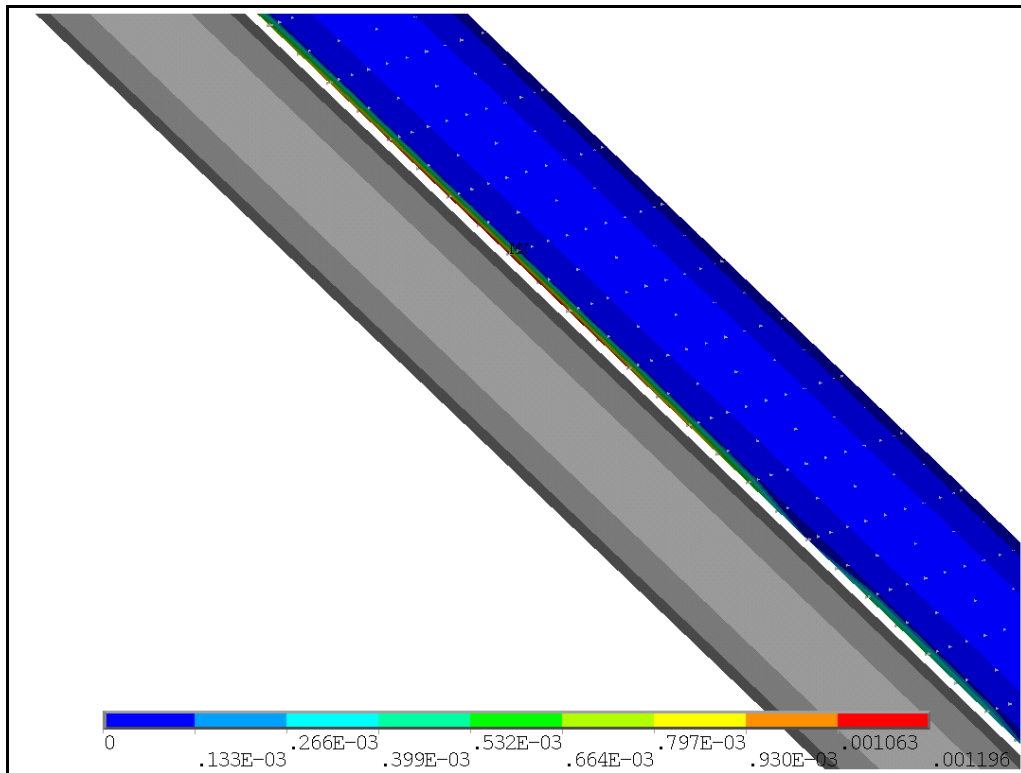


Figure 4.24: Contact Penetration

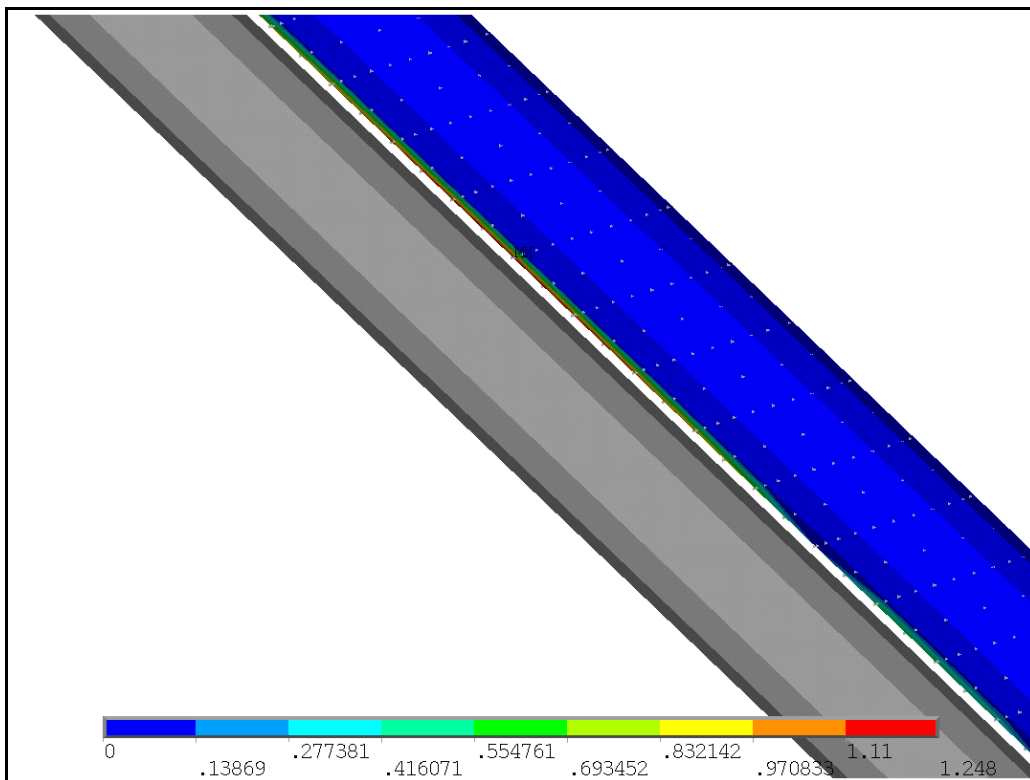


Figure 4.25: Contact Pressure

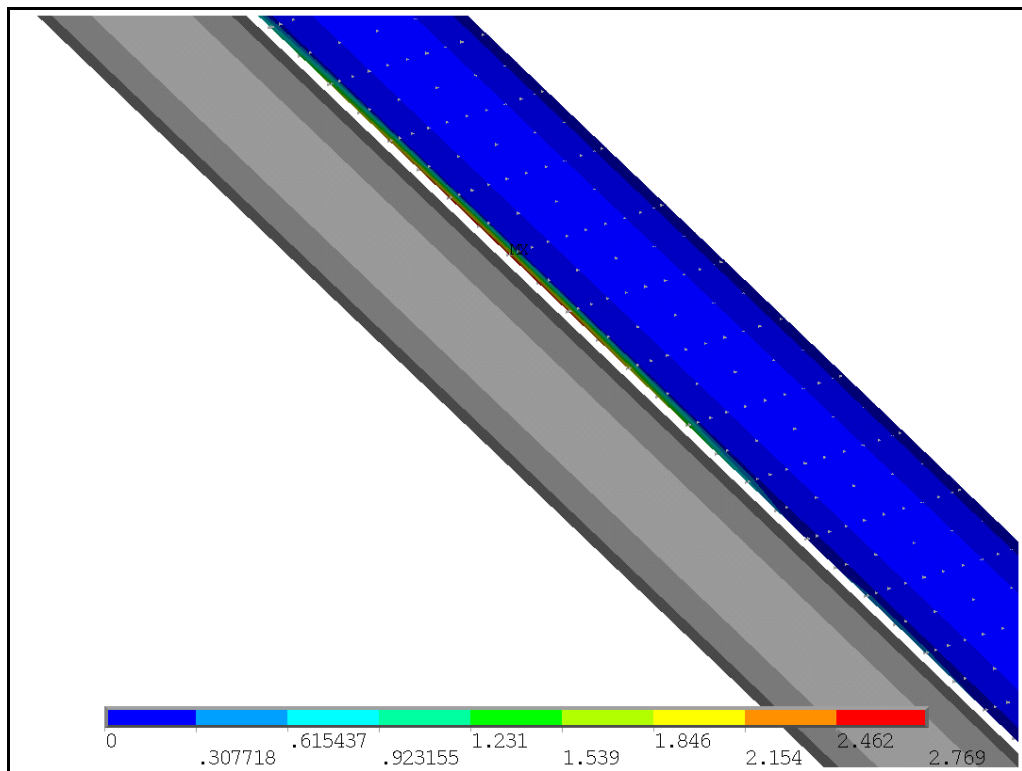


Figure 4.26: Contact Friction Stress

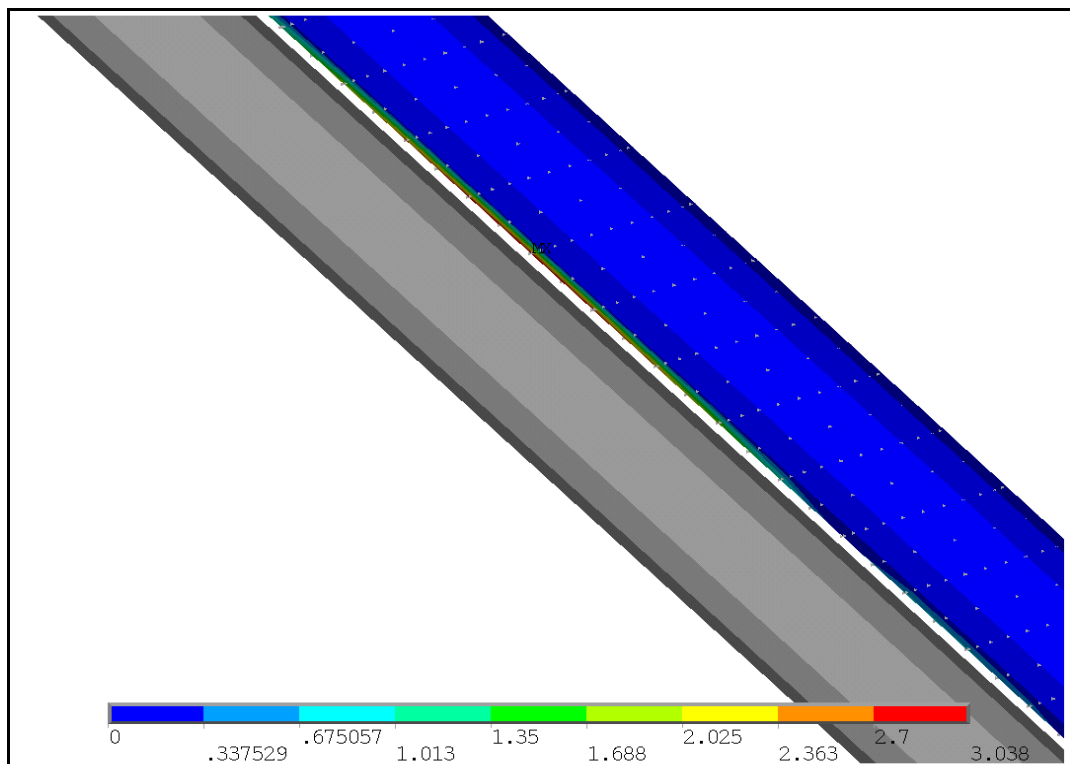


Figure 4.27: Contact Total Stress

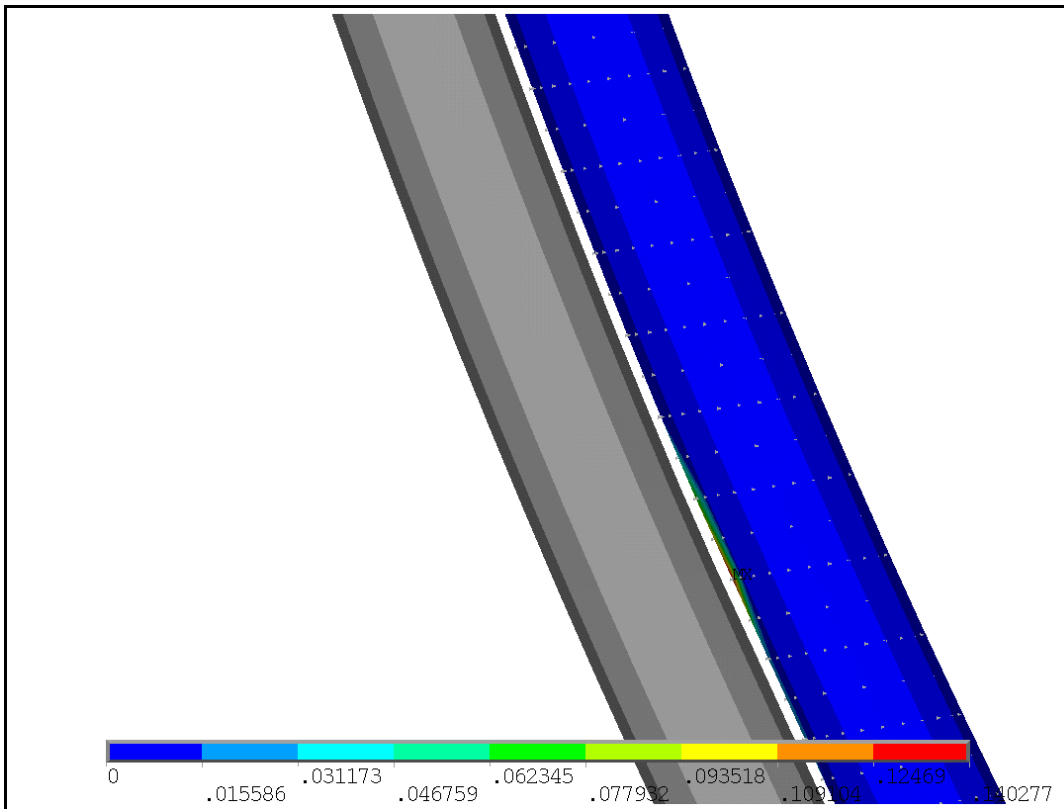


Figure 4.28: Contact Sliding Distance

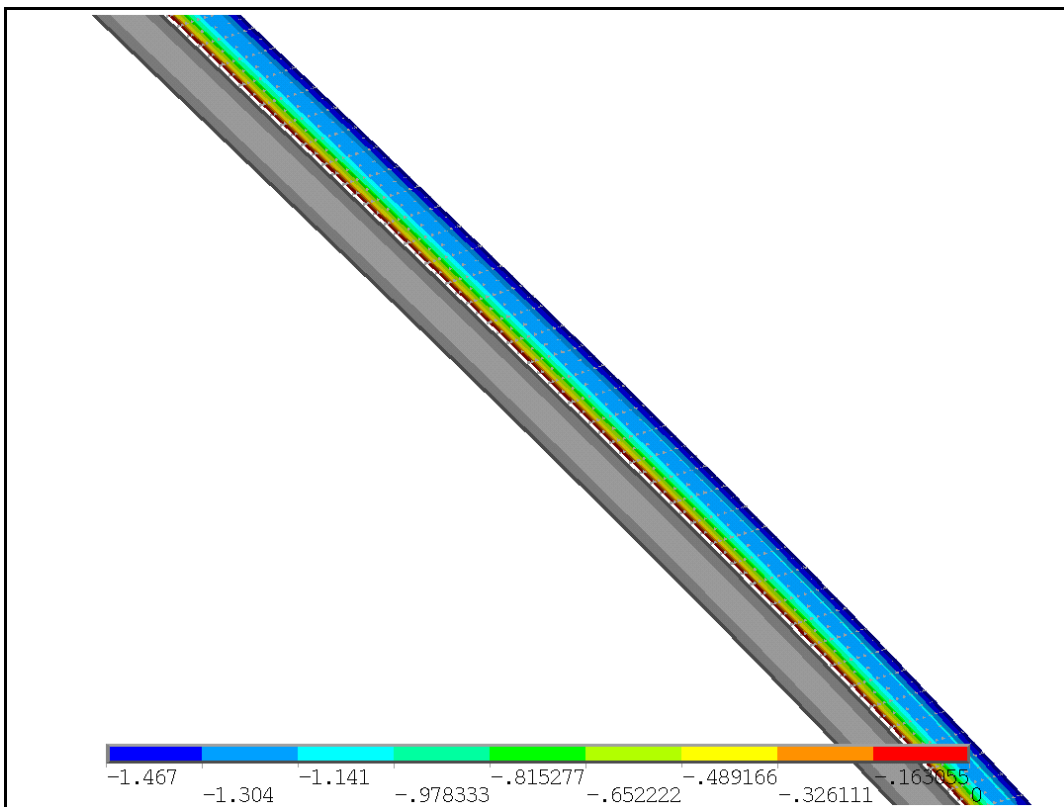


Figure 4.29: Contact Gap Distance

4.1.3 Case I.2

The Case I is a model in which carbon nanotubes are in contact after subjecting a displacement of value 50 nm in compression. The waviness ratio of carbon nanotubes is 0.2. The Boundary conditions are given in the Table 4.3.

This Case is studied in order to see the contact model contribution to the representative volume element while carbon nanotubes have an initial gap between each others. This gap value is 1 nm and the contact contribution in this model is fairly visible.

Table 4.3: Boundary Conditions

Parameters	Values
$U_z(0)$	symmetric
$U_z(250)$	-50nm
$U_y(0)$	symmetric

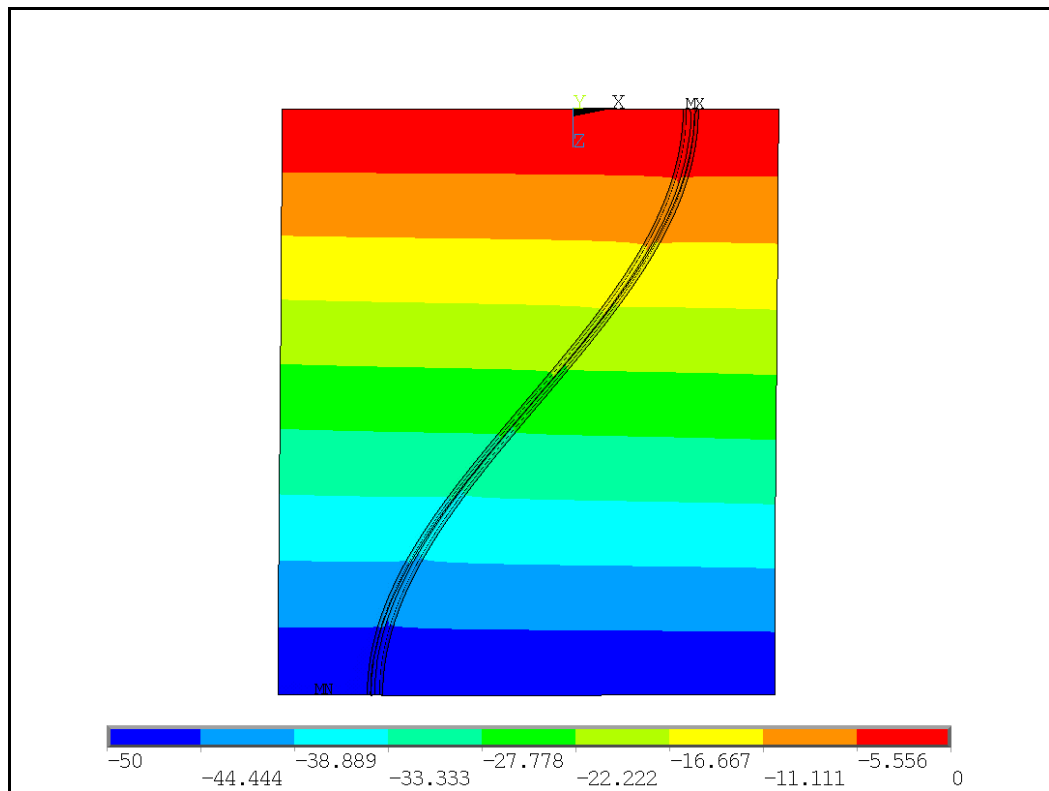


Figure 4.30: Displacement values in z direction

The contact is observed with a 50 nm displacement for the waviness ratio 0.2 as can be seen in Figure 4.30. The magnified view can be seen in Figure 4.31.

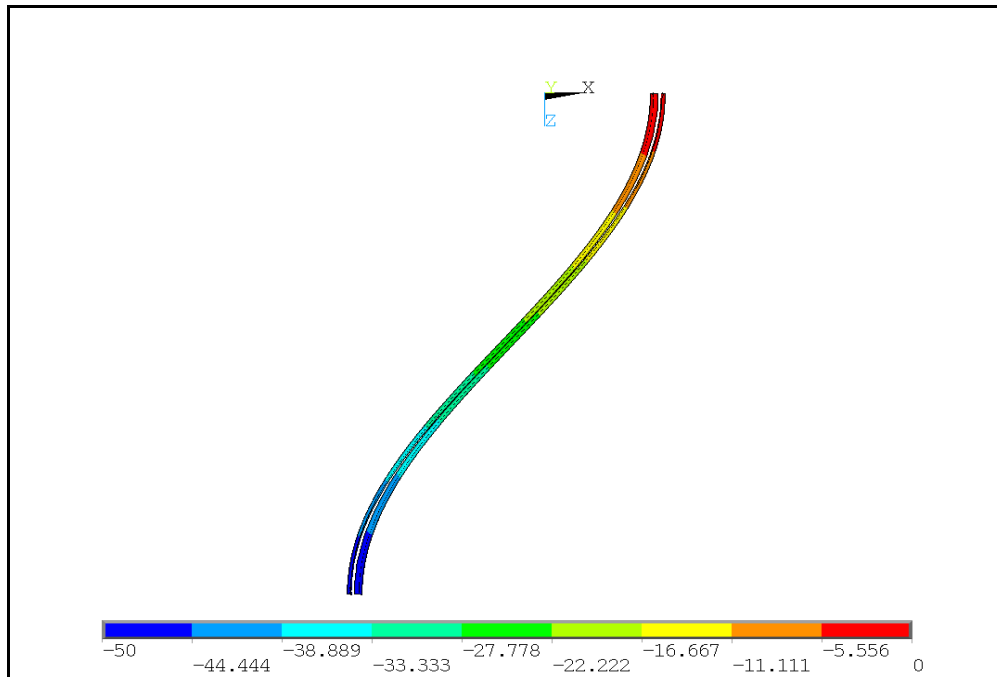


Figure 4.31: Displacement Values in z Direction (Zoomed View)

Carbon nanotubes are touching each other while displacing in the range of -33 nm to -16 nm in z direction.

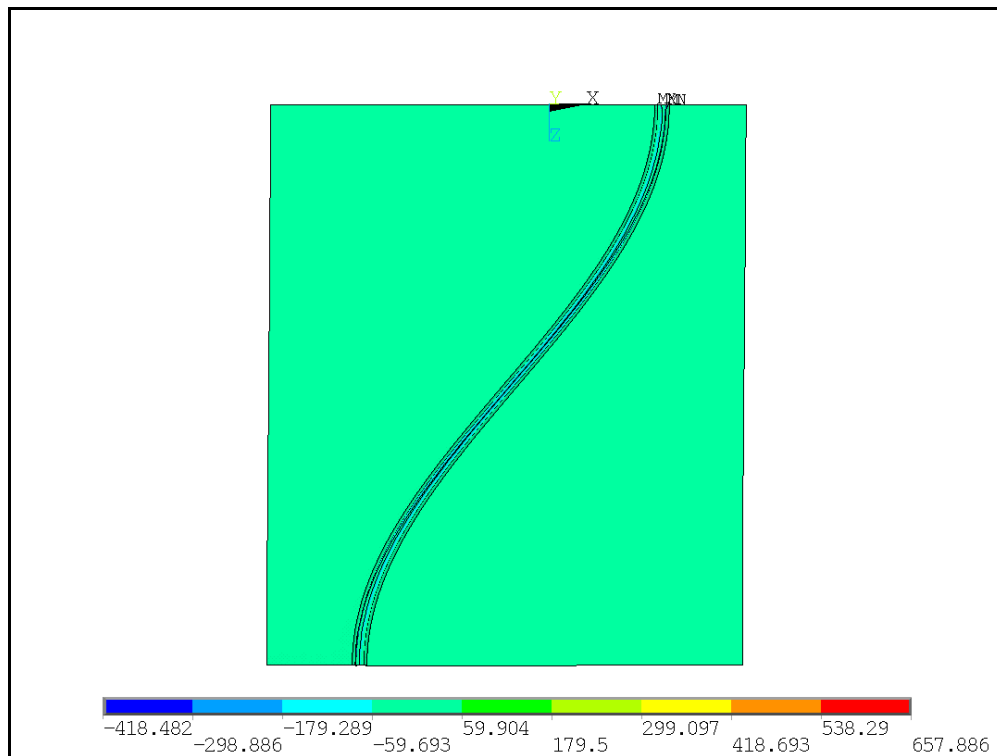


Figure 4.32: Stress Values in z Direction

The stress values in z direction is between -179.289 GPa and 59.904 GPa as can be seen in the contour scale of Figure 4.32. The maximum values is occurring in the tip points of the carbon nanotubes.

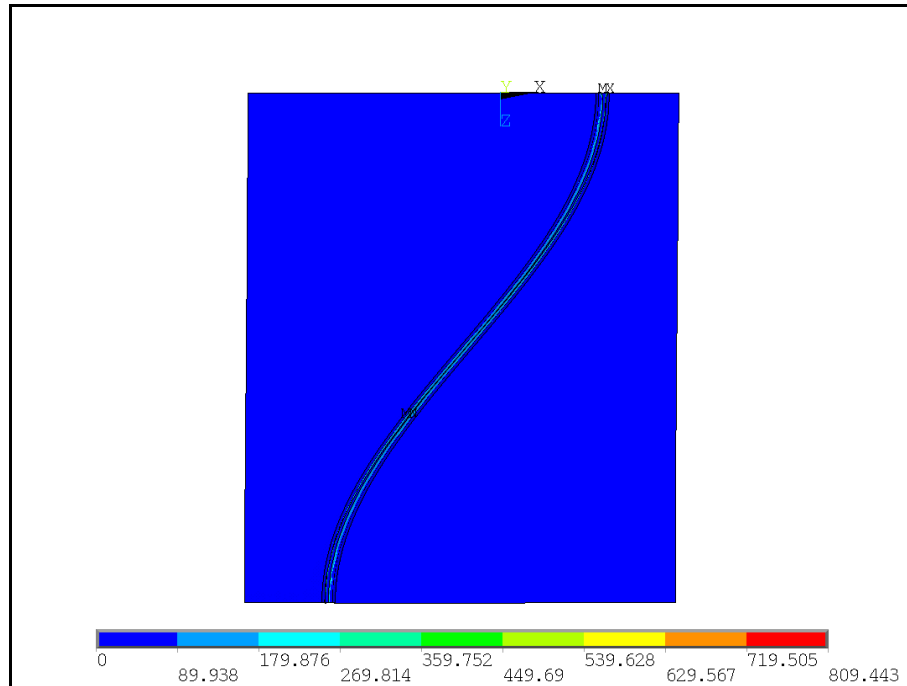


Figure 4.33: Von Mises Equivalent Stress Values

The maximum stress values are again in the tip points of carbon nanotubes. The stress values of 179-359 GPa can be seen on the carbon nanotubes in the Figure 4.33 and can be viewed in larger extent in Figure 4.34.

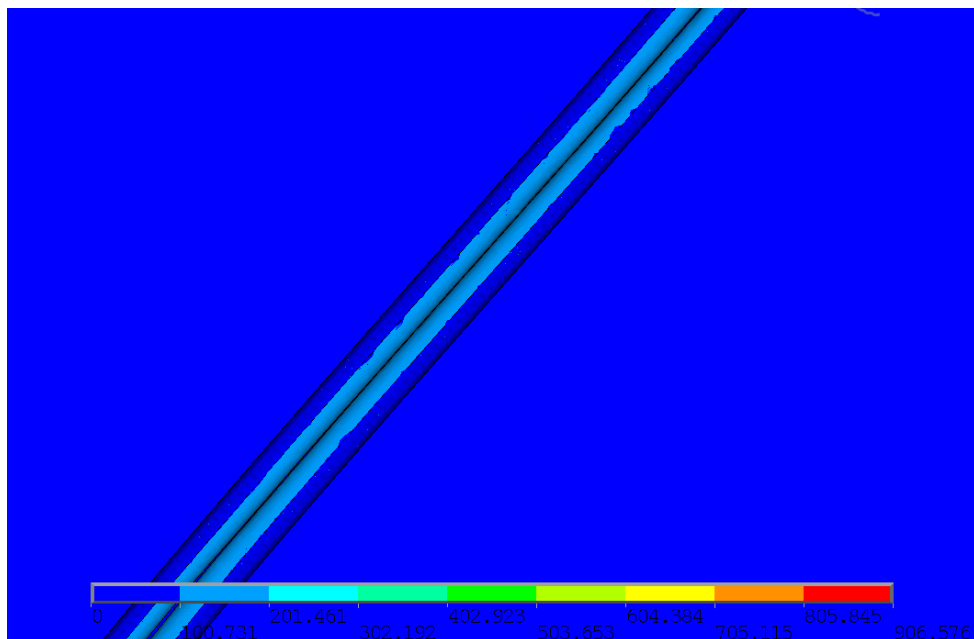


Figure 4.34: Von Mises Equivalent Stress (Zoomed View)

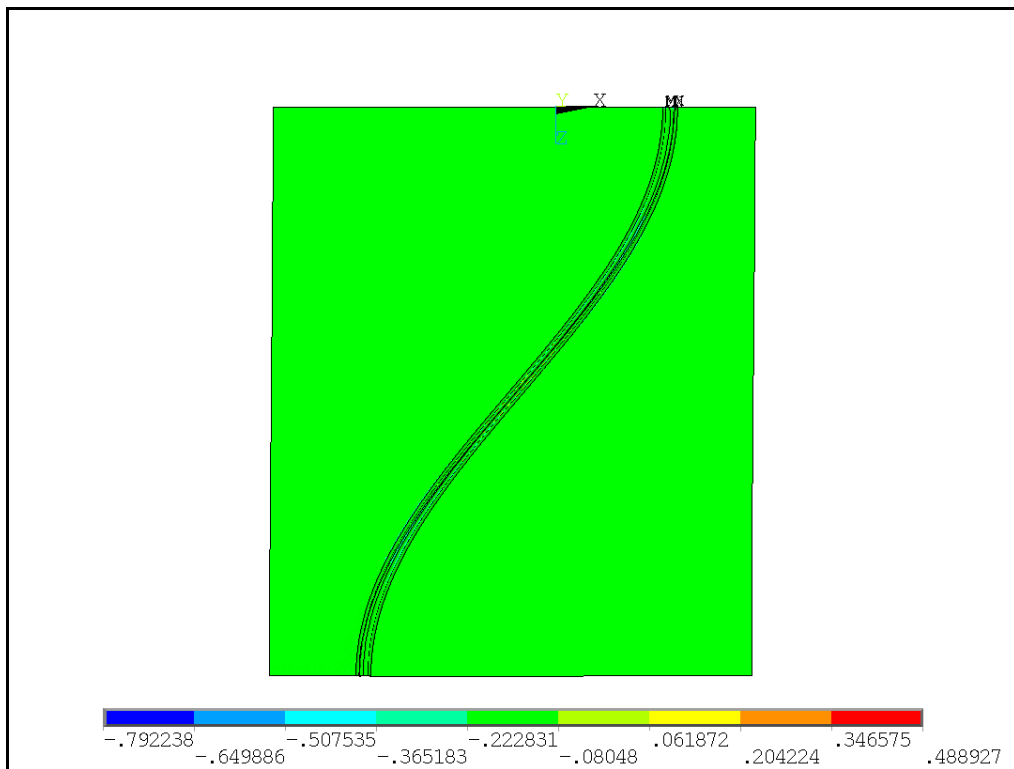


Figure 4.37: Elastic Strain in z Direction

Strain values of possible contact area are in the values of -0.25-0.069 nm scale as can be viewed in Figure 4.37 and Figure 4.38.

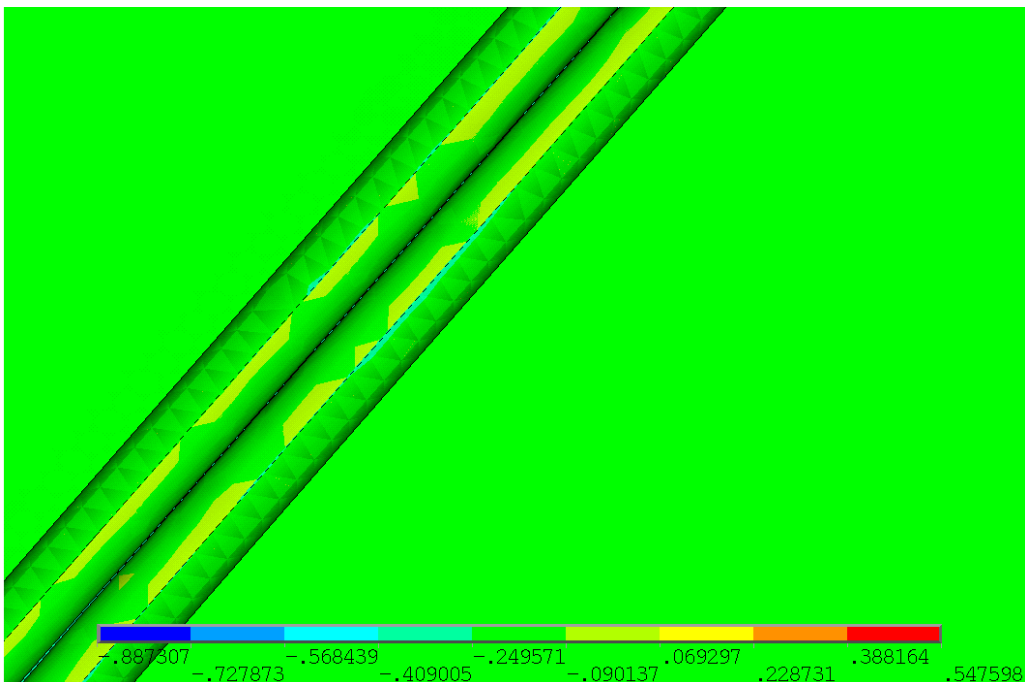


Figure 4.38: Elastic Strain in z Direction (Zoomed View)

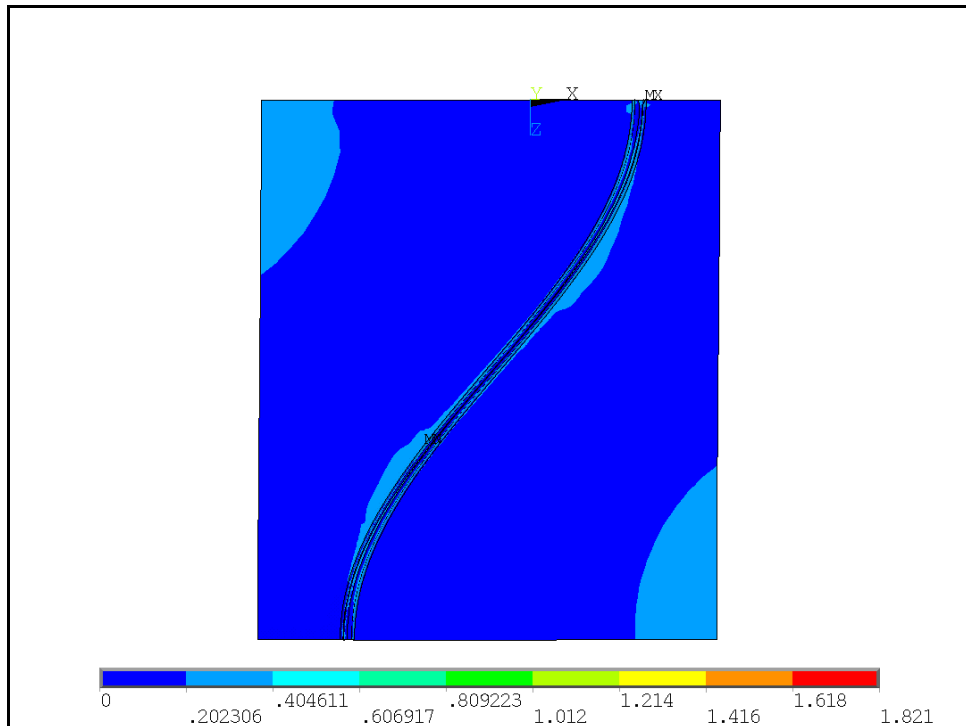


Figure 4.39: Elastic Von Mises Equivalent Strain

Elastic Von Mises strain values are in 0 nm to 0.404611 nm scale as can be seen in Figure 4.39 and Figure 4.40.

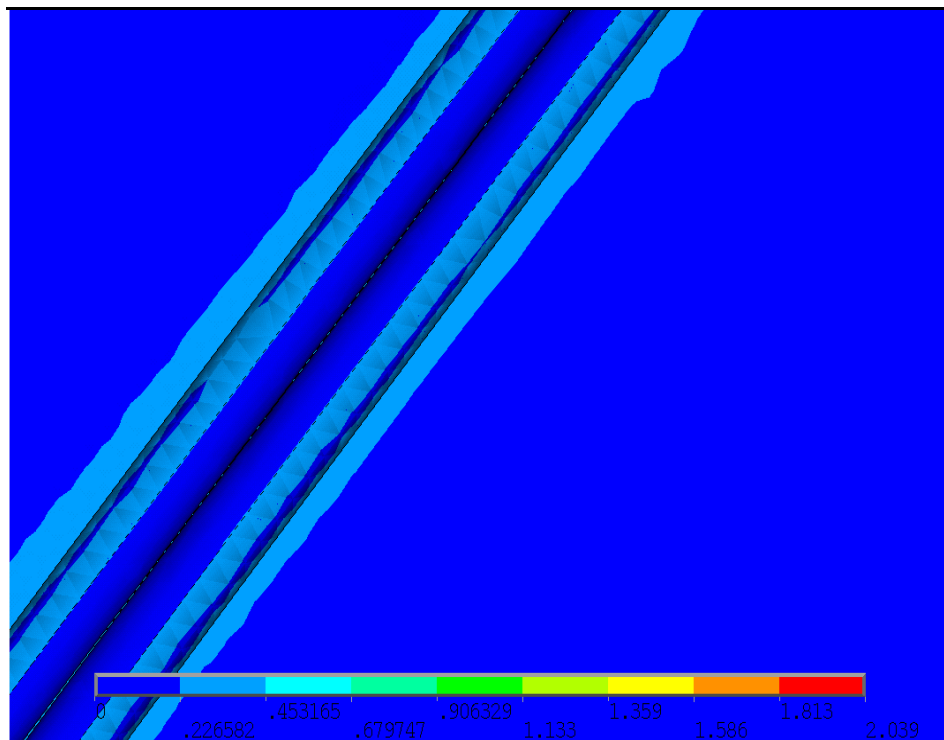


Figure 4.40: Elastic Von Mises Equivalent Strain (Zoomed View)

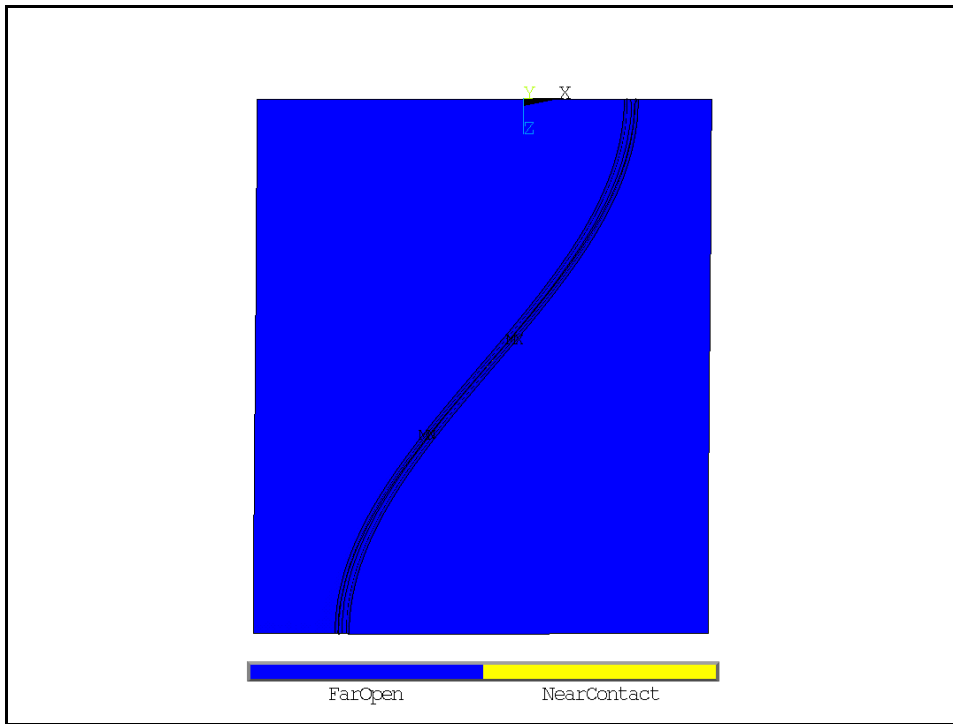


Figure 4.35: Contact Status

Contact is occurring in the center of the model as can be seen in Figure 4.35. The near contact zone is in the center of the Figure. The status can be viewed in a larger extent in Figure 4.36.

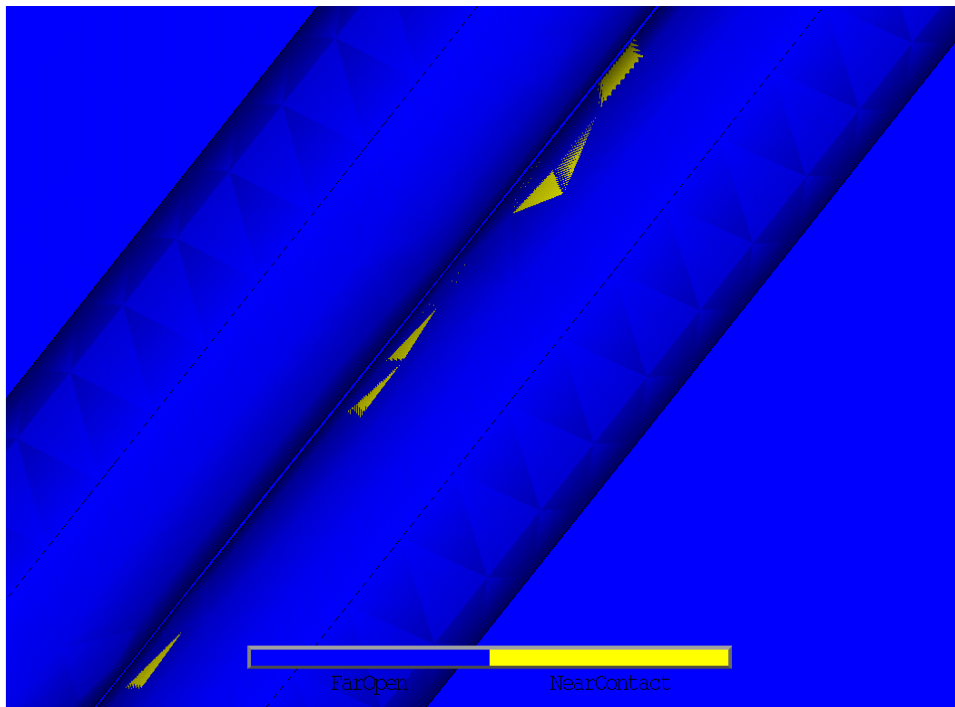


Figure 4.36: Contact Status (Zoomed View)

4.1.4 Case I.2.y

The Case I.2 is repeated in tension, the displacement in z direction is given in the Figure 4.41.

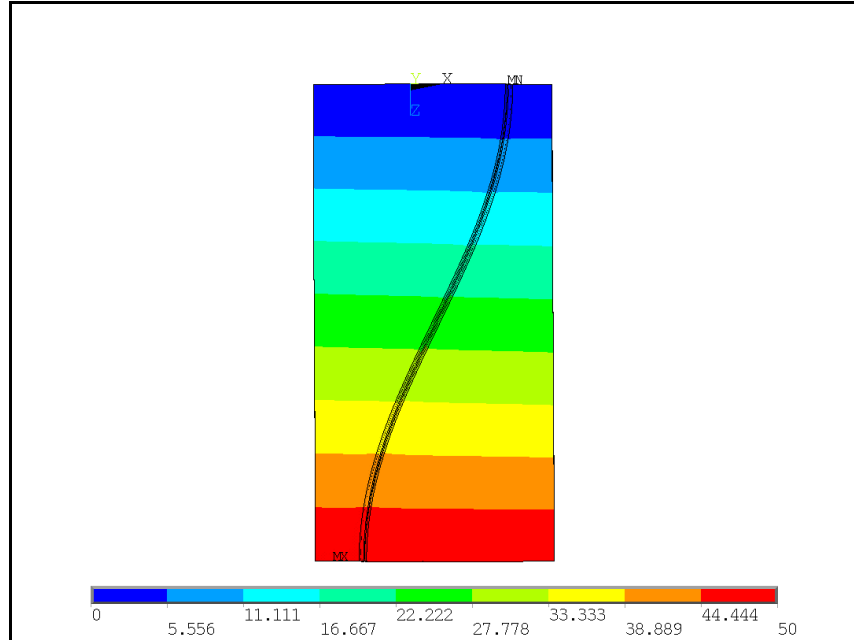


Figure 4.41: Displacement in z Direction

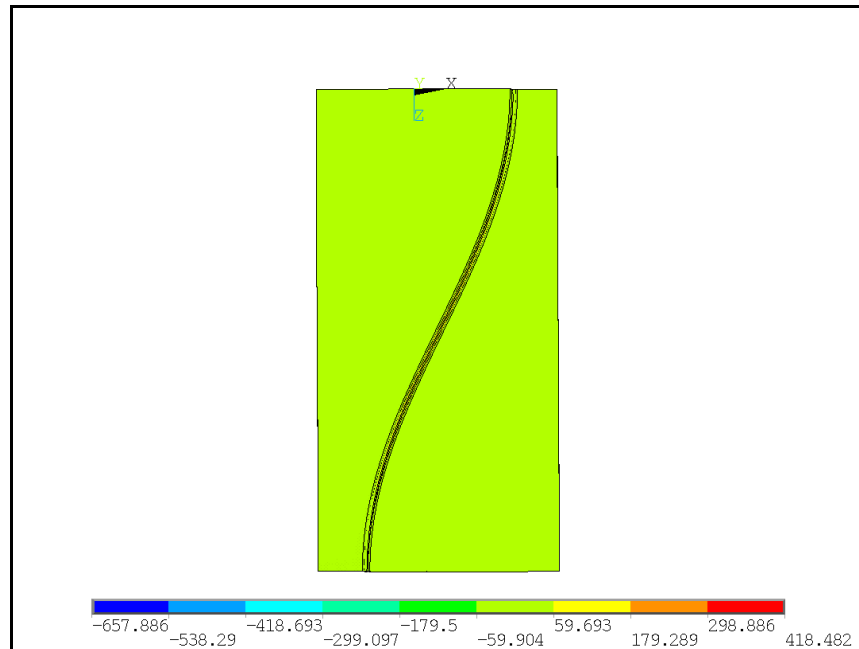


Figure 4.42: Stress in z Direction

The stress values is in z direction of -59.904 GPa to 59.693 GPa as can be seen in Figure 4.42 and in larger extent in Figure 4.43. The Elastic strains in z direction can be seen in Figure 4.44 and Figure 4.45.

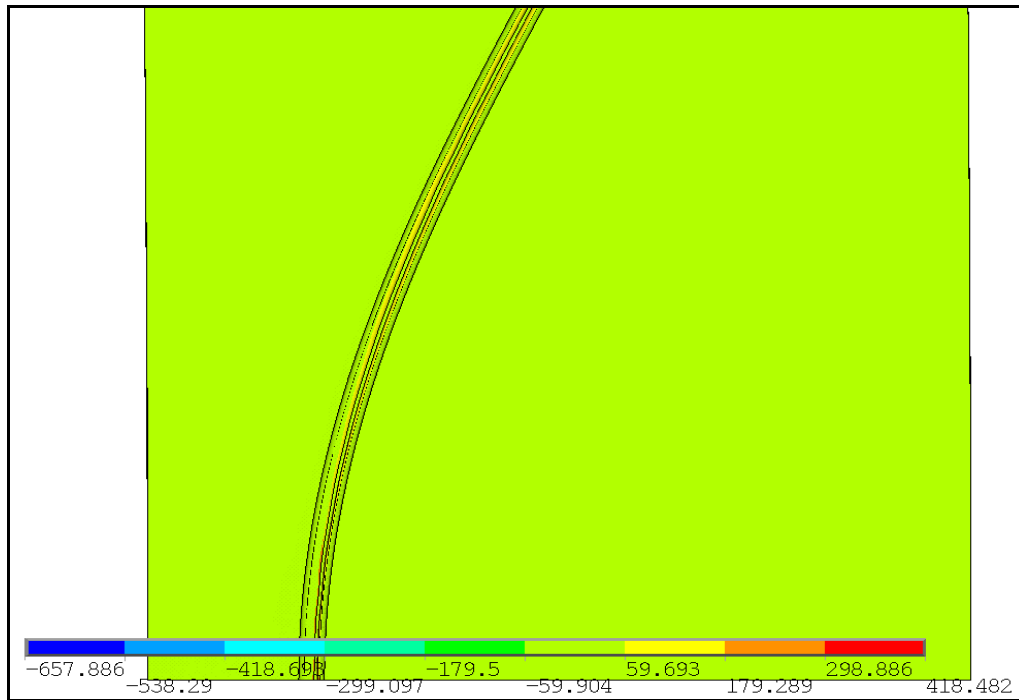


Figure 4.43: Stress in z Direction (Zoomed View)

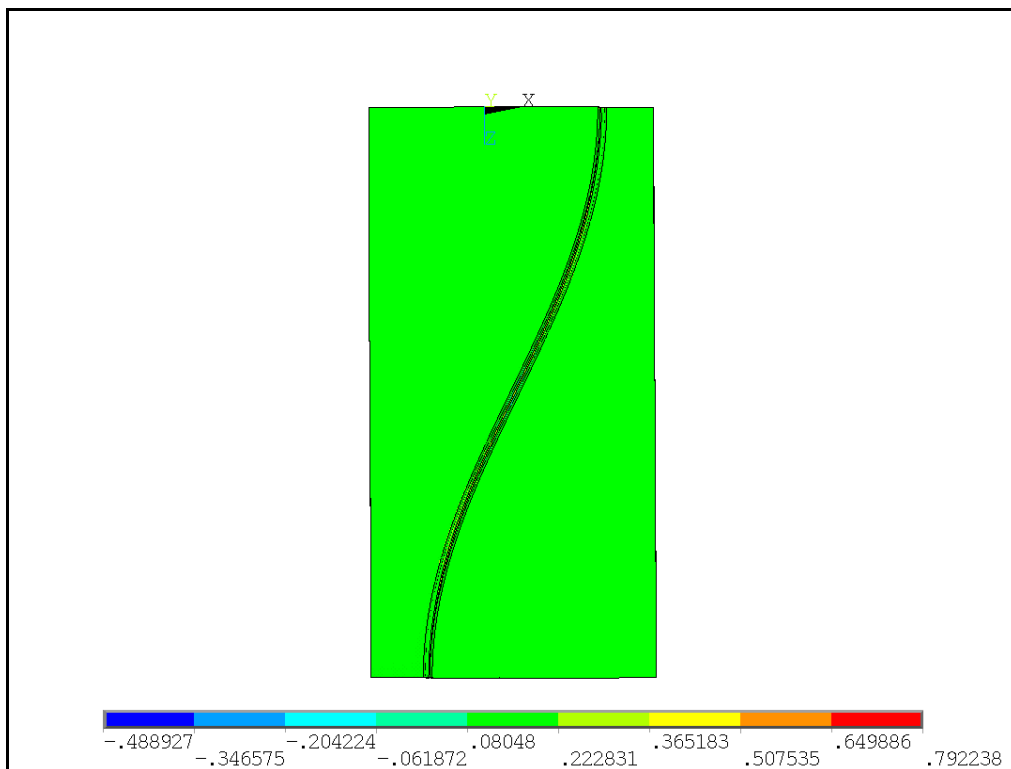


Figure 4.44: Elastic Strain in z Direction

Elastic Strain in z direction is in the values of 0.08 nm to 0.22 nm as can be seen in Figure 4.44 and Figure 4.45.

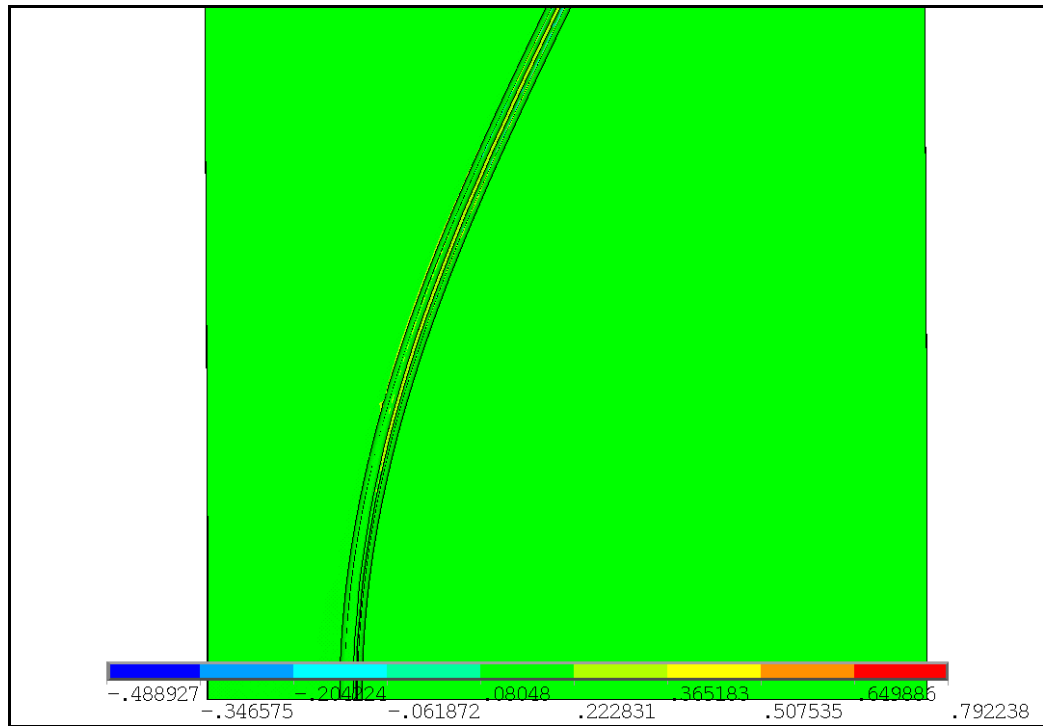


Figure 4.45: Elastic Strain in z Direction (Zoomed View)

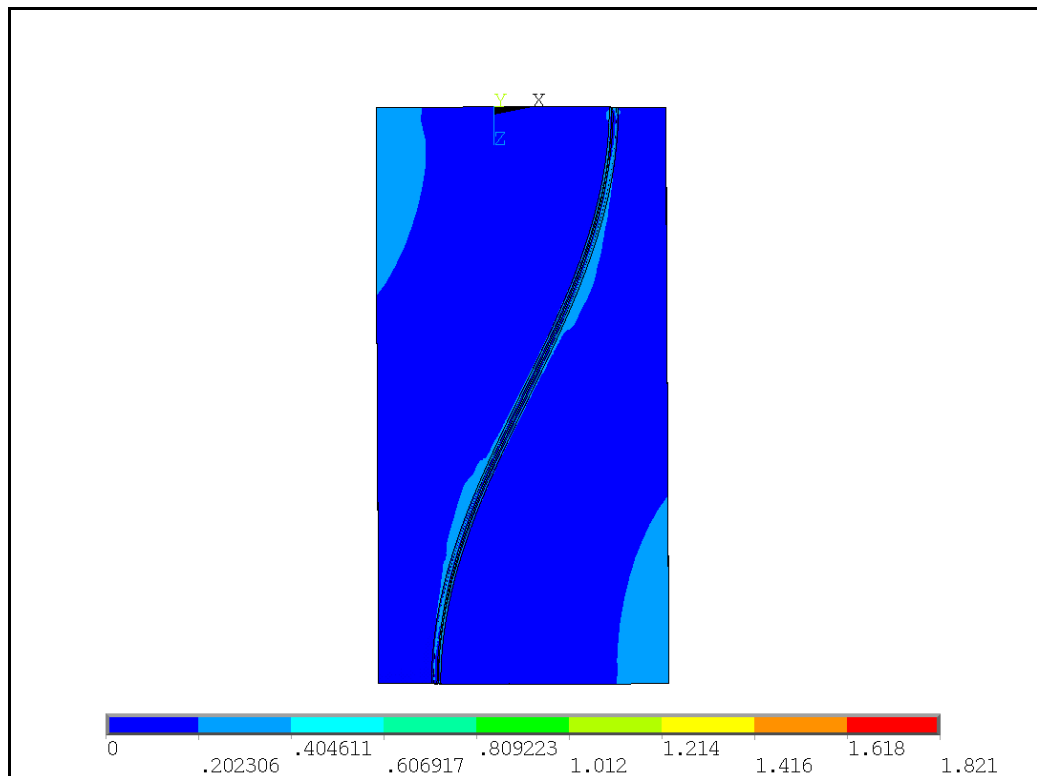


Figure 4.46: Elastic Von Mises Equivalent Strain

Elastic Von Mises Equivalent Strain are in the values of 0.40 nm to 0.6 nm. As can be seen in Figure 4.46 and Figure 4.47.

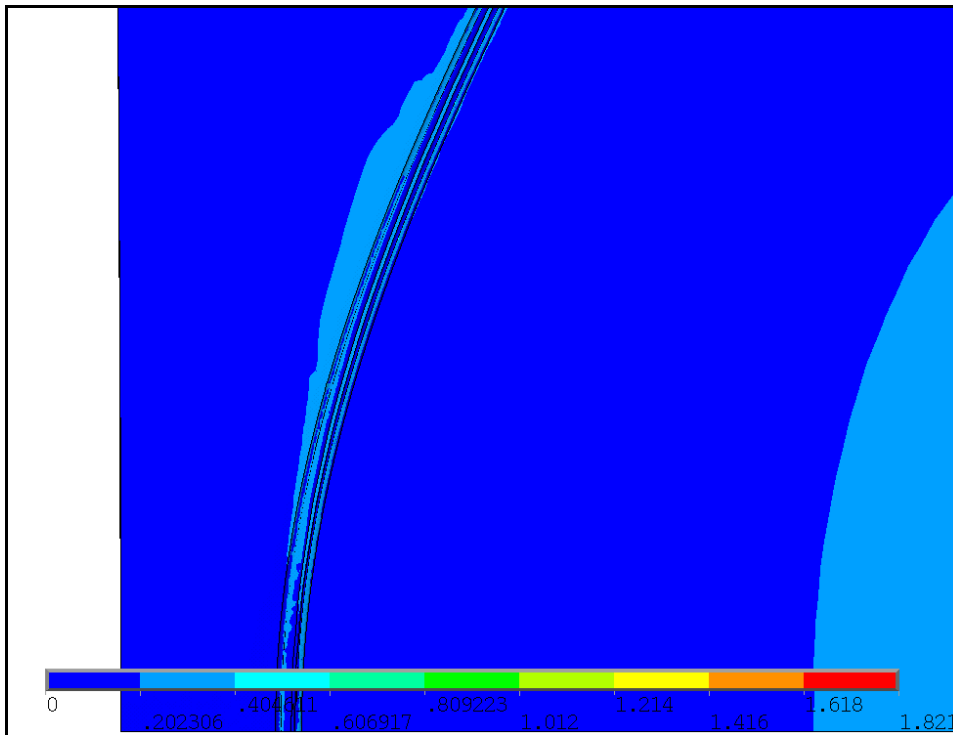


Figure 4.47: Elastic Von Mises Equivalent Strain (Zoomed View)

Contact status maximum point is near the tip of the model as can be seen in Figure 5.48.

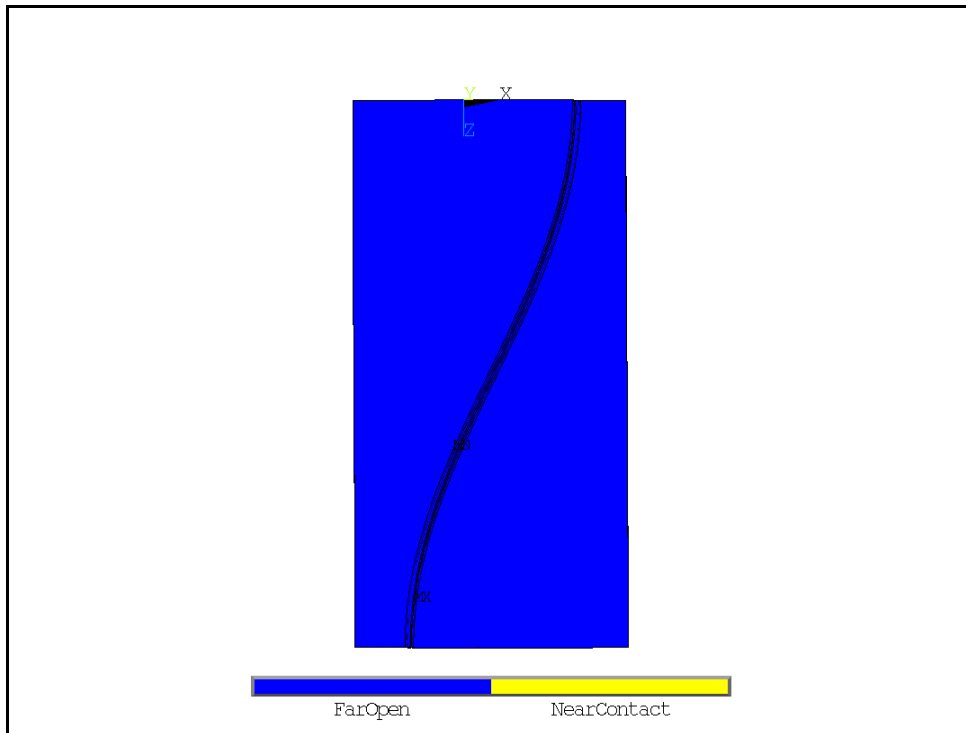


Figure 4.48: Contact Status in Tension

4.2 Case II

The geometric data is summarized in Table 4.3 and the load data is summarized in Table 4.4. And the boundary conditions are given in Table 4.5.

Table 4.4: Geometric Data

Parameters	Values
Carbon Nanotube Aspect Ratio	0.008
Carbon Nanotube Waviness Ratio	0.3
Representative Volume Element Aspect Ratio	1.54

4.2.1 CaseII.1

The Case II is modeled with an initial contact where the boundary conditions are given in Table 4.4.

Table 4.5: Boundary conditions for Case II.1

Parameters	Values
Uz(0)	symmetric
Uz(250)	-20 nm
Uy(0)	symmetric

Displacement of 20 nm is given on face of the y-z plane of the model as can be seen in the Figure 4.49. Von Mises Equivalent Stress Elastic Stress as can be seen in Figure 4.50 and in larger extent in Figure 4.51. The Von Mises Equivalent Elastic Strains can be seen in Figure 4.52 in the order of 0 to 0.13 nm which changing with the nanotube curvature.

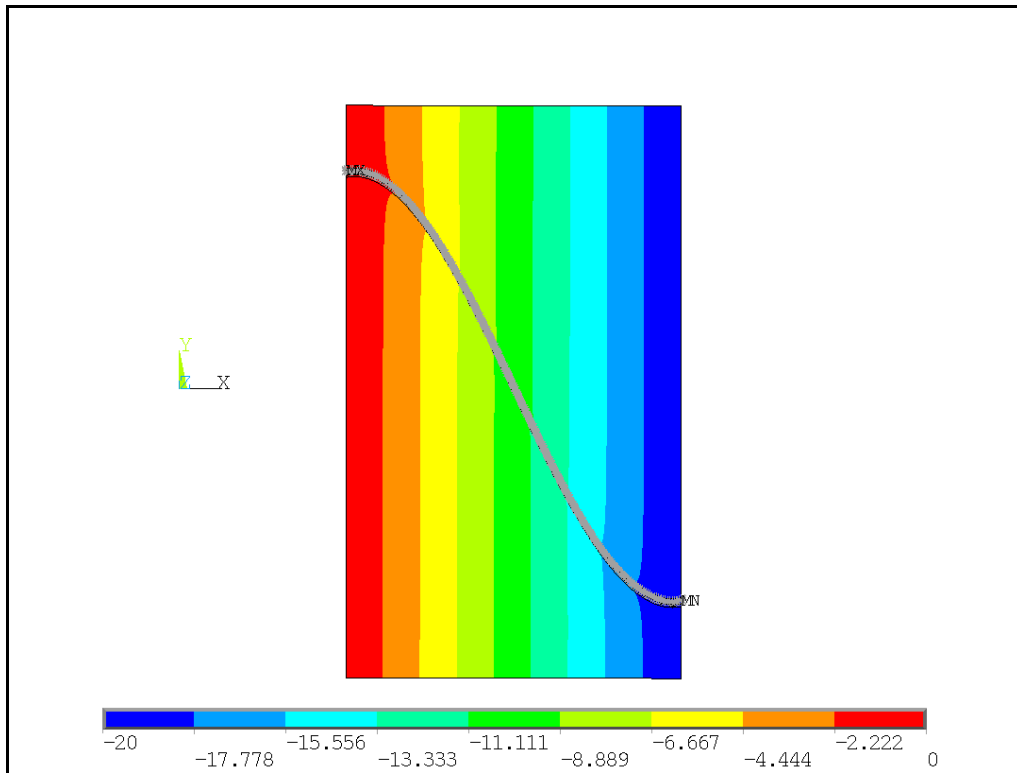


Figure 4.49: Displacement in x Direction

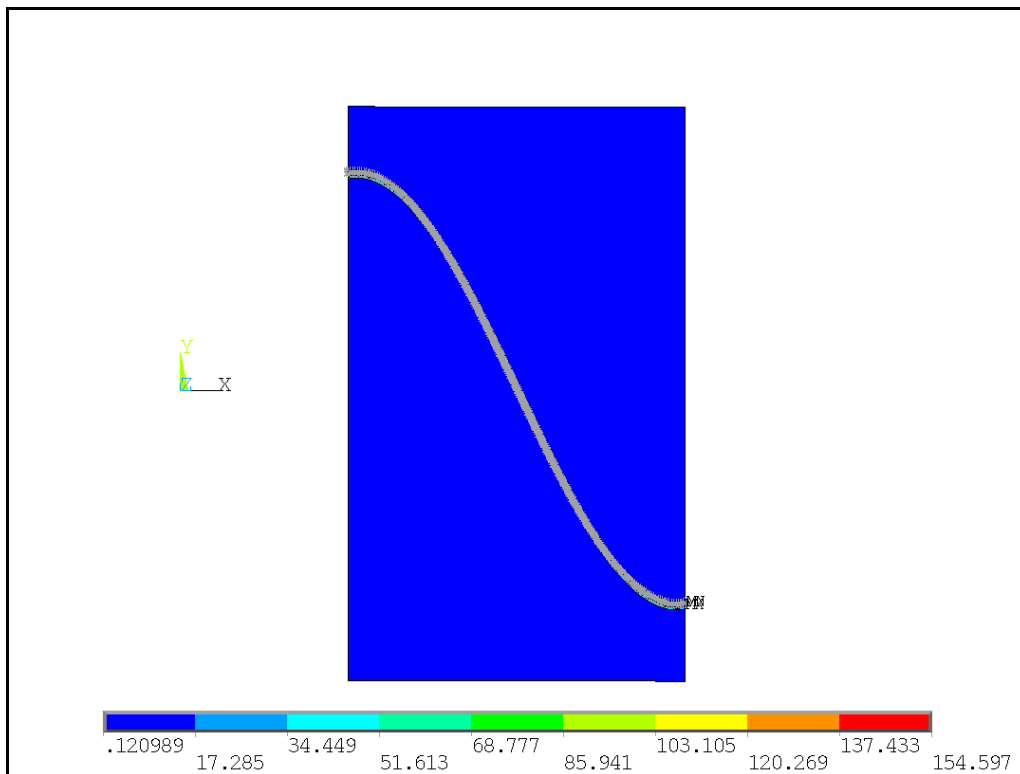


Figure 4.50: Von Mises Equivalent Stress

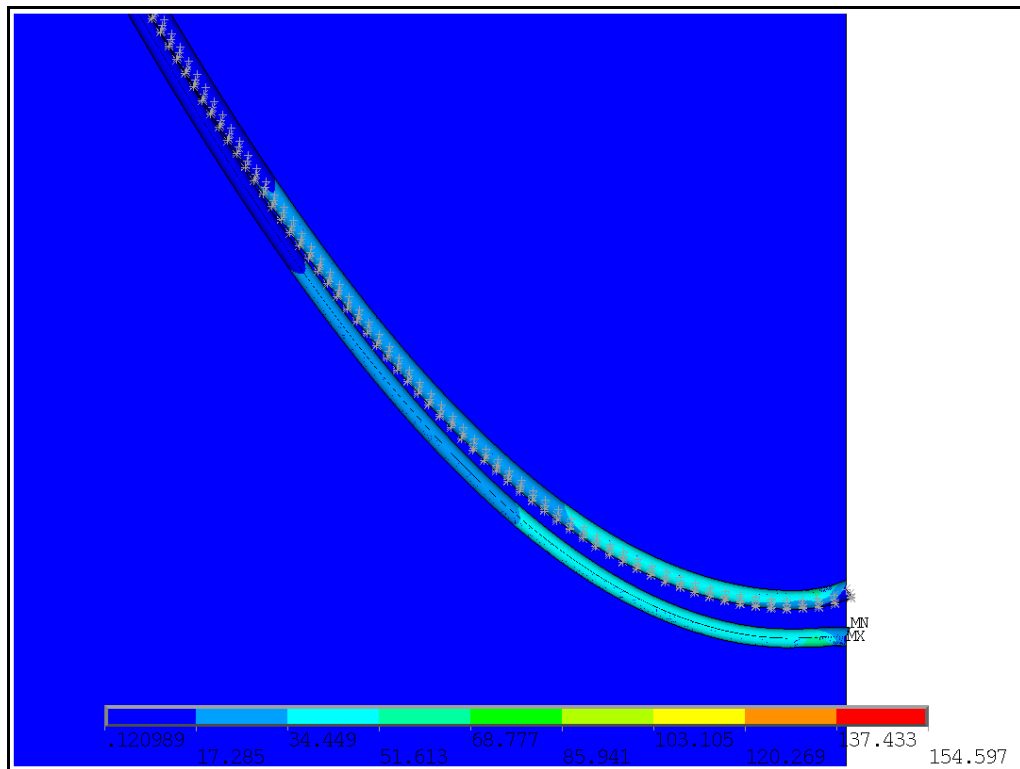


Figure 4.51: Von Mises Equivalent Elastic Stress (Zoomed View)

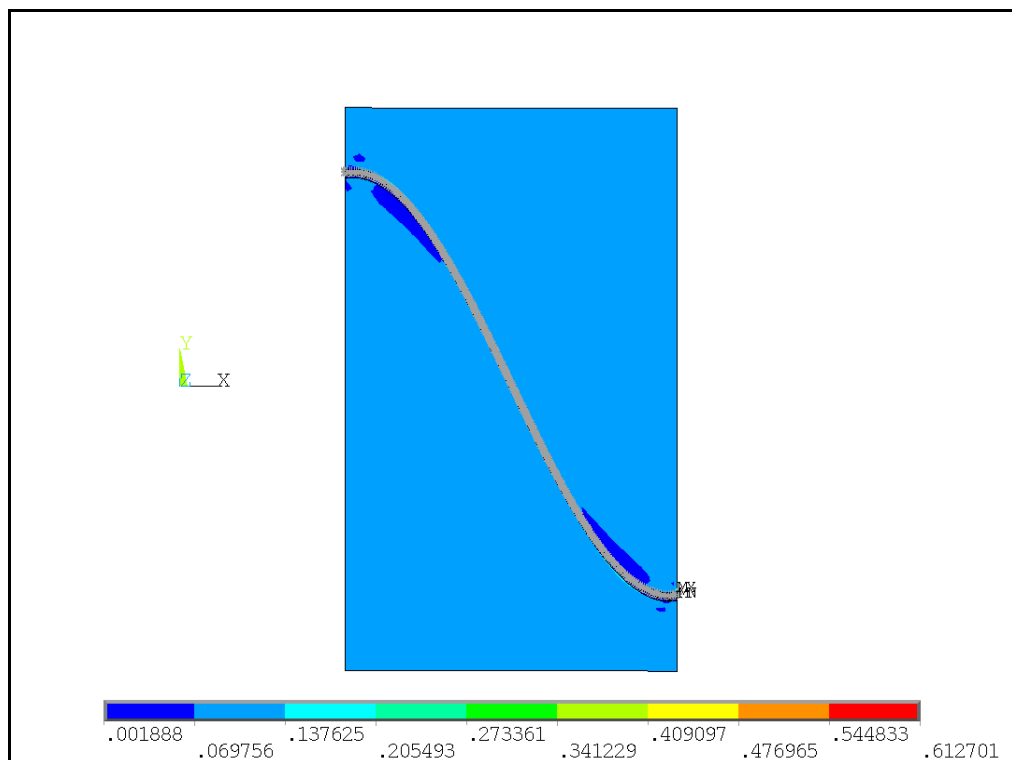


Figure 4.52: Von Mises Equivalent Elastic Strain

Sticking and sliding contact is occurred in the middle of the mode as can be seen in the contact status in Figure 4.53 and in larger extent in Figure 4.54.

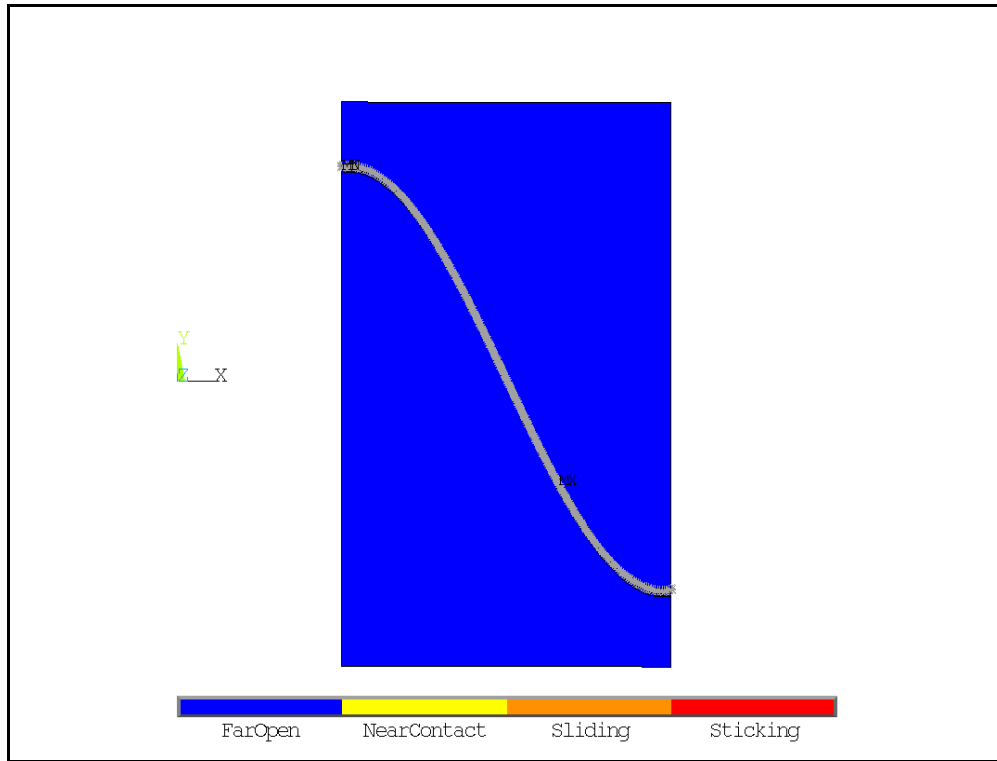


Figure 4.53: Contact Status

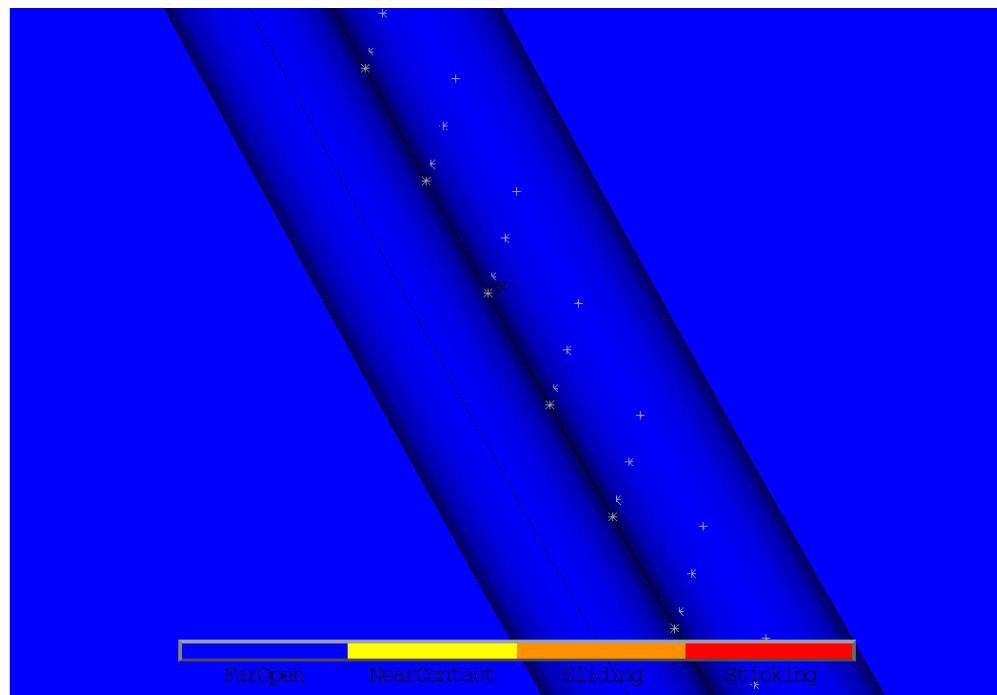


Figure 4.54: Contact Status of Carbon Nanotubes

4.2.2 Case II.1.x

The Case II.1 is modeled with only carbon nanotubes using the same boundary condition's data in the Table 4.5. This study was made in order to see the

contribution of the epoxy matrix in the representative volume element model to the mechanical contact interaction between the carbon nanotubes. The epoxy matrix is probably restricting the carbon nanotubes displacement. This is one of the difficulties occurring in the contact model. The numerical results can be seen in Figure 4.55 to Figure 4.58.

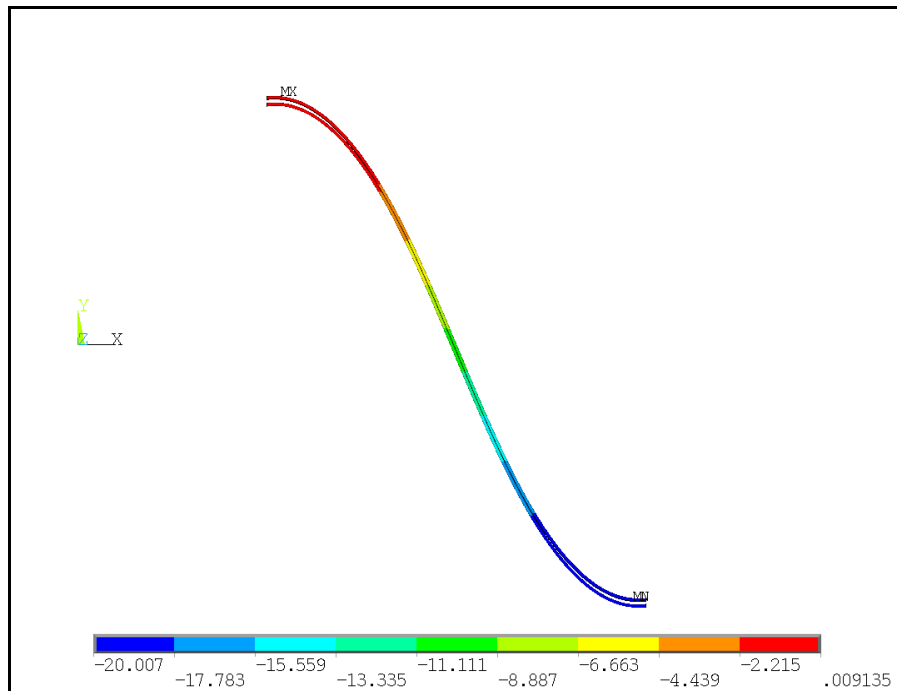


Figure 4.55: Displacement in z Direction

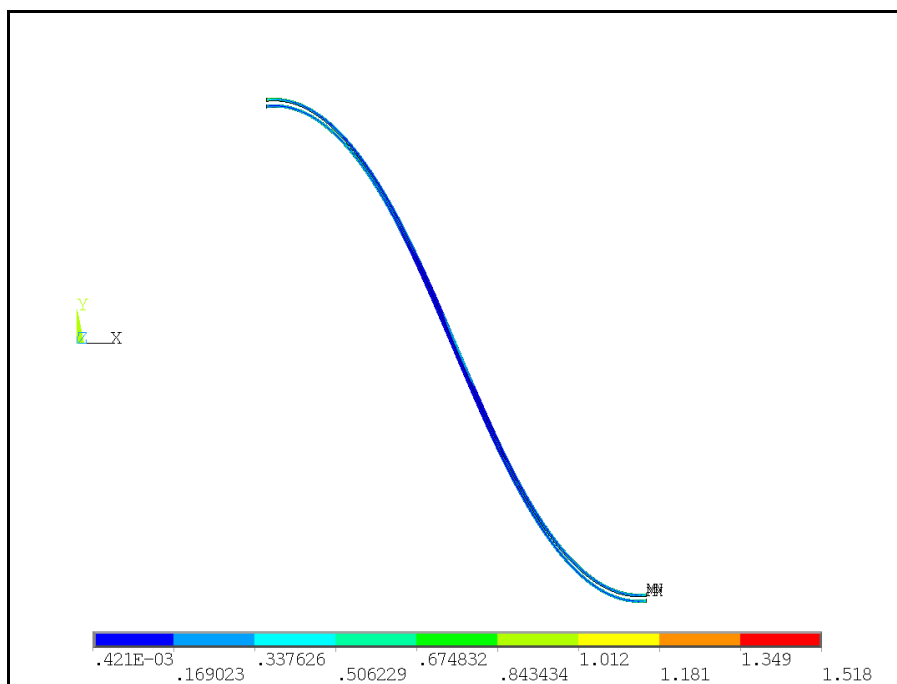


Figure 4.56: Von Mises Equivalent Elastic Stress

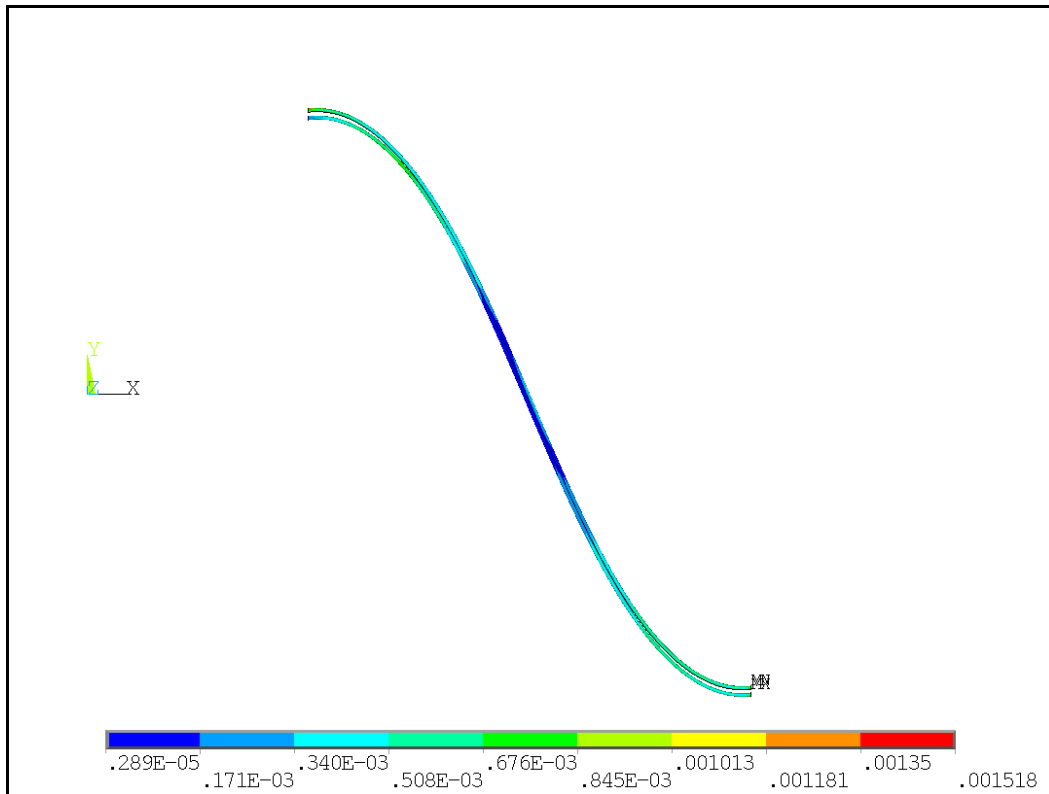


Figure 4.57: Von Mises Equivalent Elastic Strain

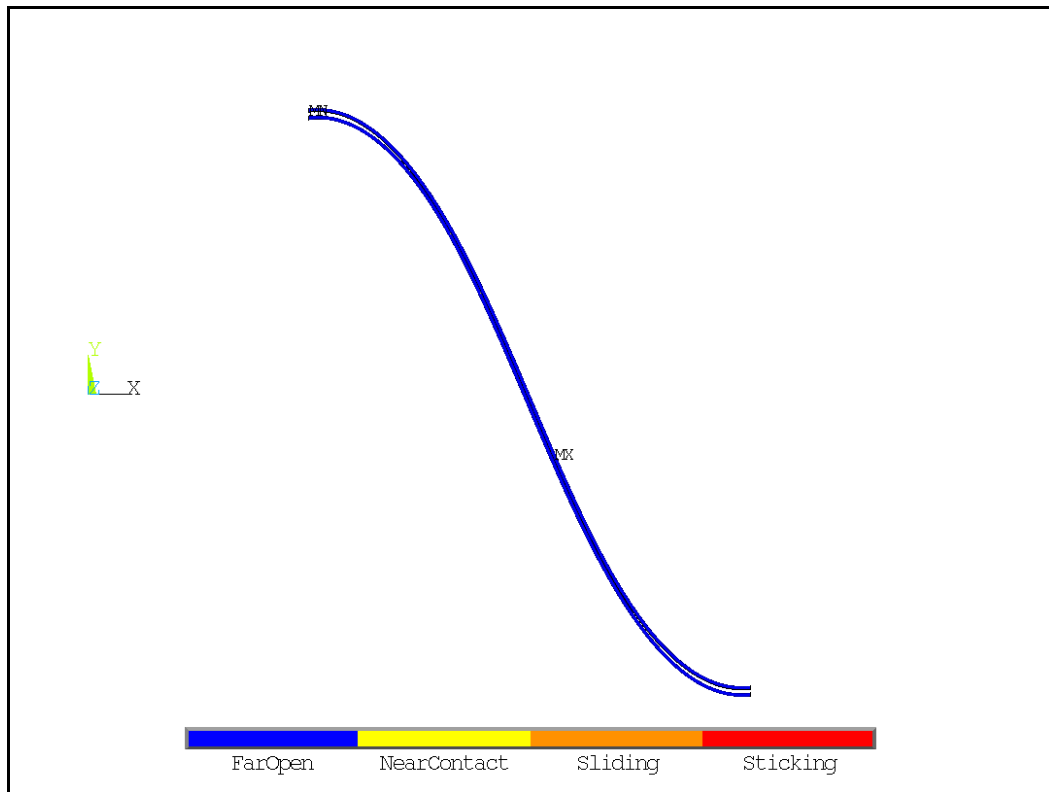


Figure 4.58: Contact Status

4.3 Comparison of Cases

The global elastic modulus can be calculated via a well-know formulas from strength of materials,

$$E = \frac{P.L}{\delta.A} \quad (4.1)$$

where P is the total reaction force in the direction of the displacement, δ is the displacement, L is the length of the representative volume element without consideration of curvature effect and A is the cross sectional area give in Table 4.6.

Table 4.6 : Cross sectional areas of the models

Area	Values (nm ²)
Case I	19998.3155
CaseII	19996.5655
Case “x”	2.136

Case I.1, Case II.1 and Case “x” numerical results with and without contact models are given in Table 4.6.

Volume of epoxy is $4.99 \times 10^6 \text{ nm}^3$ and volume of carbon nanotube (considered straight) is 1570 nm^3 . The volume ratio of carbon nanotubes,

$$V_f = \frac{V_{\text{CNTs}}}{V_{\text{CNTs}} + V_{\text{EPOXY}}} \quad (4.2)$$

And volume faction of carbon nanotubes considered as straight form is $V_f = 0.000314$. Global elastic modulus from the rule of mixtures,

$$E = V_f E_{\text{CNT}} + (1 - V_f) E_{\text{epoxy}} \quad (4.3)$$

$E = 5.312 \text{ GPa}$ is the global modulus without taking into consideration contact and waviness effects.

The model numerical results can be seen in Table 4.7 and Table 4.8. The more reliable results are obtained for the case I.1 in the Table 4.7. While for the Case I.2 due to contact model difficulties, the numerical results are not representative. Because of the initial gap of 1 nm between carbon nanotubes in the model, contact integration points did fairly overlap with each other and some convergence problems

occurred. Far contact and near contact status are occurred in the model. The reasons of this problem may depends on many factors such as inadequate constraint definitions, fewer integrations points...etc. The model solutions can be more practically obtained in Ansys LS-DYNA® module. However this was an irrelevant way for this thesis and more effort was done for model case I.1 in which initial gap is not used.

Table 4.7: Reaction Forces and Global Elastic Modulus of the Case I.1 and II.1 of Representative Volume Element and Model with Only Carbon Nanotubes.

		Representative Volume Element	Elastic Modulus Difference (%)	Only Carbon Nanotubes (Case “x”)	Elastic Modulus Difference (%)
Case I.1	With Contact	Rz=8046 nN E=5.0292 GPa		Rz=0.10969 nN E=0.6418 GPa	
	Without Contact	Rz=8021.4 nN E=5.0138 GPa	0.31	Rz=0.03855 nN E=0.2256 GPa	7.96
Case II.1	With Contact	Rz=7703.5 nN E=4.8155 GPa		Rz=0.01089 nN E=0.0637 GPa	
	Without Contact	Rz=7700 nN E=4.8133 GPa	0.046	Rz=0.12173 nN E=0.7123 GPa	-

In the Table 4.8, the Case I which is a model in which carbon nanotubes are in contact after subjecting a displacement of value 50 nm in compression is compared between the models with contact and the without contact contribution.

Moreover the results of the case named “y” which is the loading of the Case I in tension can be seen in Table 4.8. As can be seen from the elastic modulus differences between the contact and the without contact cases, the contact model are not appropriate in these cases due to contact model difficulties. Thus their results in Table 4.8 did not taken into consideration in the conclusions.

Table 4.8: Reaction Forces and Global Elastic Modulus of the Case I.2 Case “y” with and without contact.

		Compression	Elastic Modulus Difference (%)	Tension (Case “y”)	Elastic Modulus Difference (%)
Case II.2	With Contact	Rz=8054.7 nN E=5.034 GPa		Rz=8054.7 nN E=5.034 GPa	
	Without Contact	Rz=8054.7 nN E=5.034 GPa	0	Rz=8046.8 nN E=5.034 GPa	0

5. CONCLUSIONS AND FUTURE WORKS

In this study, the effect of the contact occurring between the two neighboring carbon nanotubes and the matrix modeled as a square representative volume element via finite element method.

Elastic modulus by rules of mixtures with the filler volume fraction without considering contact and waviness effect is 5.12 GPa which is 1-2% higher than the elastic modulus of with and without contact cases with two different waviness ratios.

This was a predictable results because as explained before carbon nanotube waviness have an adverse effect to the strength of the material. In other words while waviness ratio increases, the global elastic modulus decreases.

The most important fact obtained was to see the contact contribution as a strength enhancement mechanism from the Model Case I.1 in which carbon nanotubes have 0.2 waviness ratio and there was any initial gap between them. Results gived 0.3% stiffness enhancement to the global elastic modulus observed due to interaction effect.

In this thesis mechanical interaction between carbon nanotubes effect is studied. Supplementary, multiphysical interaction effect can be studied to observe physical interaction effect to the global elastic modulus of the material.

Future projects can be done in order to expand the results obtained. Model Case I.1 can be a fundamental step and results can be repeated for different displacements' values in order to obtain a statistical result. The model will be developed by using molecular dynamics approach in which atomic effects will be included.

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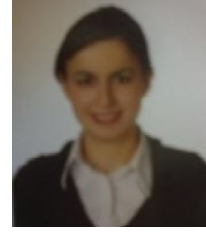
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CURRICULUM VITAE



Name Surname: Beril AKIN

Place and Date of Birth: Izmir, 25 November 1985

E-Mail: berilyumakn@gmail.com

B.Sc.: Celal Bayar University, Mechanical Engineering, 2008