# Prediction of mechanical properties of EPON 862 (DGEBF) cross-linked with curing agent (TETA) and SiO 2 nanoparticle based on materials studio

**Article** *in* IOP Conference Series Materials Science and Engineering · December 2018

DOI: 10.1088/1757-899X/454/1/012139

CITATIONS
0

READS
17

**1 author:**

Nuha Hadi Jasim Al Hasan
University of Basrah
**7** PUBLICATIONS **0** CITATIONS

SEE PROFILE

**PAPER** • **OPEN ACCESS**

# Prediction of mechanical properties of EPON 862 (DGEBF) cross-linked with curing agent (TETA) and $SiO_2$ nanoparticle based on materials studio

To cite this article: N H J Al Hasan 2018 *IOP Conf. Ser.: Mater. Sci. Eng.* **454** 012139

IOP Conf. Series: Materials Science and Engineering **454** (2018) 012139 doi:10.1088/1757-899X/454/1/012139

# Prediction of mechanical properties of EPON 862 (DGEBF) cross-linked with curing agent (TETA) and $SiO_2$ nanoparticle based on materials studio

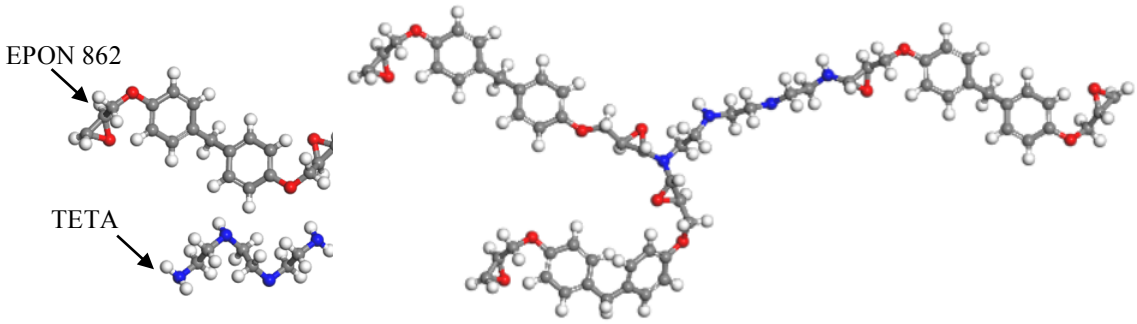
**N H J Al Hasan**[1]

[1] Department of Engineering Material, College of Engineering, University of Basrah, Iraq

**Abstract**. The present study focuses on the prediction of mechanical properties of $SiO_2$ nanocluster reinforced epoxy resin (DGEBF) cross-linked with curing agent W (TETA). The MD models of the reinforced epoxy were built using the amorphous module of Material Studio 7.0 (Accelrys Inc.). The mechanical properties of this cross-linked structure were determined using MD simulations. $SiO_2$ qurtiz with different aspect ratios of weight percent (6%, 8% and 10%) in order to construct amorphous unit cells of $SiO_2$-Epoxy nanocomposites. The $SiO_2$-Epoxy nanocomposites system undergoes NPT (constant number of atoms, pressure and temperature) ensemble with applied uniform strain field during MD simulation to obtain density curve, cell size diagram and the results file.

## 1. Introduction

The aerospace epoxy resin EPON 862 produced by Hexion Specialty Chemicals Inc. is good mechanical properties for composite applications. Two reactive sites exist in the EPON 862 monomer, during cross-linking process either one or both of these reactive sites of EPON 862 create new bonds with any of the four reactive sites in Triethylenetetramine TETA (nitrogen groups red ball groups) hardener when they come close enough to each other within a certain distance[1] ,as shown in Figure 1. The ball-and-stick model of the cross-linked epoxy repeat unit is built by Materials Studio software, typical amorphous cross-linked epoxy network consists of 3 EPON 862 neat resin molecules and TETA curing agent molecules, Make the cross-linked epoxy as basic material.




a. EPON 862 and TETA (curing agent) b. the cross-linked epoxy

**Figure 1.** Molecular model of a. EPON 862 and TETA (curing agent) b. the cross-linked epoxy

The EPON 862 is very strong due to its tight linkage due to highly crossing linked polymer chains that form an irreversible network structure, this material is categorized as a thermosetting polymer, it is relatively brittle with low stiffness [2]. When mixing EPON 862 with the hardener, curing of the resin is achieved. Based on molecular mixture calculations with a cure ratio of 3:1, three molecules of resin combine with one molecule of the curing agent.

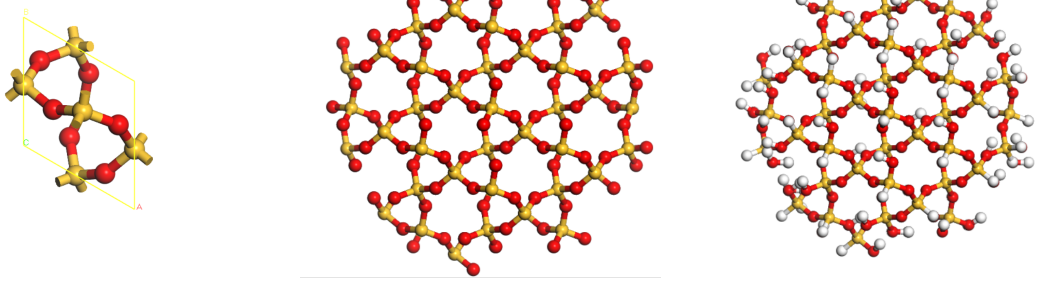
An extensive literature review was undertaken for EPON 862 cured with TETA by molecular dynamics (MD) simulation, from MD simulations low crosslink density of the epoxy resin voids and impurity inside the epoxy compound may result in the degraded material properties studied by Rai A K , Amit Porwal A and Mishra S B [3], Kim B.ChoI J.,Yu S., Yang S. and Cho M.et al Investigated the effects of crosslink densities on thermo-mechanical properties of thermoset polymeric nanocomposites via molecular dynamics (MD) simulations in the study of [4],they conclusion that the presence of more crosslinks in polymer matrix interphase are weakened.

Arab B, Shokuhfar A [5] utilized the molecular dynamics with COMPASS, PCFF, UFF and Dreiding force fields for calculation of the material properties of cross-linked epoxy polymers, it is results that the COMPASS and PCFF can be reliably used for simulation of cross-linked polymers with calculation of their properties.

## 2. Simulation details

### *2.1. $SiO_2$ nanopartical embedded in epoxy amorphous cell:*

By Material Studio 7.0 (Accelrys Inc.), the geometry optimization via Smart method using the Forcite Module for modeling Silica crystals model. Then Sphere with the radius of the particles was set to 10A$^{o}$, was selected from the build nanocluster dialog. When click the build button for construction a nanocluster, a silicon nanoparticle with many unsaturated bonds of Si and O on the surface was obtained as shown in Figure 2.(a) , all of the unsaturated bonds adjust Hydrogen button for simulate the real process of oxidation[6]. $SiO_2$-nanoparticle without unsaturated bonds is shown in Figure 2(b).



a- **$SiO_2$** qurtiz

b- **$SiO_2$-nanoparticle with unsaturated bonds**

c- **$SiO_2$-nanoparticle with saturated bonds**

**Figure 2.** $SiO_2$-nanoparticle model

### *2.2. Amorphous unit cell with cross-linked epoxy polymer:*

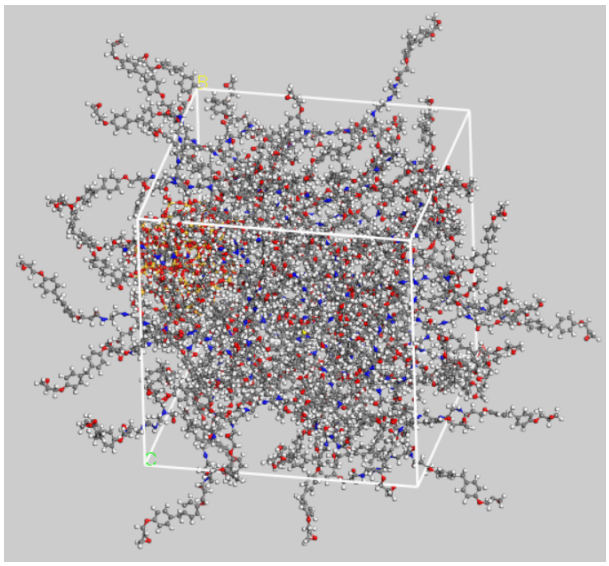
MD simulation was conducted in unit cells consisting of cross-linked EPON 862 resin. A typical amorphous unit cell contains epoxy-curing agent in the ratio of 3:1 was used. For defining the bonded and non-bonded interactions, (Compass II) force field was used. A brief description of simulation is provided below:

The $SiO_2$ nanopartical were embedded in the three-dimension periodic amorphous unit cells for evaluating bulk elastic properties. In this study, 6%, 8% and 10% of $SiO_2$ nanopartical by weight was considered in the amorphous unit cell, the results shown in Figure 3. The density of amorphous $SiO_2$ nanoparticle -epoxy unit cells was kept in the range of not exceeds 1.0 gm/cc. However, this changes

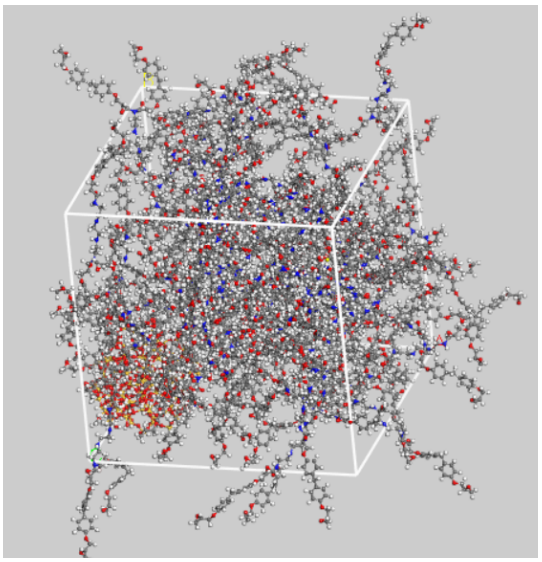
during the molecular dynamic equilibration process. The number of epoxy monomers was determined in such a way which ensures expected weight percentage of $SiO_2$ nanoparticle in the unit cell. Table 1 shows material configurations with relevant $SiO_2$ nanoparticle aspect ratio and weight percentage:

**Table 1.** Number of epoxy molecules and $SiO_2$ in a unit cell

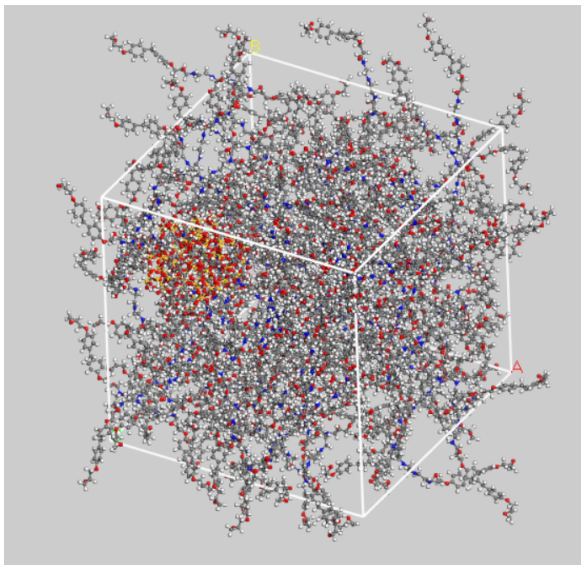
| Material Configuration | Weight percentage of SiO2 | Number of Epon molecules Unit cell | Unit cell dimension ($A^0$) |
|---|---|---|---|
| I | 6% | 101 | a=b=c=57.7 |
| II | 8% | 74 | a=b=c=52.4 |
| III | 10% | 58 | a=b=c=48.7 |



a epoxy/6%SiO2



b. epoxy/8%SiO2 8%



c. epoxy/6%SiO2 10%

**Figure 3.** Unit Cell Model of epoxy/SiO2 at different weight percent

## 3.Mechanical Properties Simulation

Select Modules| Forcite| Calculation to open the Mechanical Properties dialog. The appropriate precision is set and other parameters are kept the default values. The relevant information of the initial parameters, the stiffness matrix and flexibility matrix of the composite, by Reuss, Voigt and Hill formula respectively, bulk modulus and shear modulus was are calculated, Lame constants and the stress along X ,Y and Z direction are obtained from the calculation results files.

The nano-particle reinforced polymer matrix composite is considered as the anisotropic material on microscopic view, while on macro-level is close to isotropic material. So it can be assumed the material is close to isotropic. For isotropic material, the stress-strain relations can be described by two constants Lame λ and μ, which can be expressed as [7]:

$\lambda = \frac{1}{3}(C_{11} + C_{22} + C_{33}) - \frac{2}{3}(C_{44} + C_{55} + C_{66})$ …… (1)

$\mu = (C_{44} + C_{55} + C_{66})$ …… (2),

The common elastic parameters can be expressed by these equations:

$\nu = \frac{\lambda}{2(\lambda+\mu)}$ …… (3) , $E = \mu\left(\frac{3\lambda+2\mu}{\lambda+\mu}\right)$ …… (4),

$K = \lambda + \frac{2}{3}\mu$ , …… (5) $G = \mu$ …… (6)

## 4. Results and discussion

### *4.1. Mechanical Properties Comparison and Analyses*

$SiO_2$-epoxy amorphous unit cells were subjected to molecular dynamic equilibration under NPT ensemble (constant number of atoms, pressure and temperature) for 5000 thousand steps of simulation with 1.0 fs time step and temperature of 298 K with 1.0 atm pressure. In order to equilibrate the internal pressure of the system and obtain a stable volume [8]. the results of elastic stiffness matrix are shown in Table 2.

**Table 2.** The elastic stiffness matrix of epoxy/$SiO_2$ unit cell

| 6% weight $SiO_2$ | | | | | | |
|---|---|---|---|---|---|---|
| *Cij* (GPa) | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 4.2565 | -5.5280 | -0.1391 | 1.1747 | 2.5311 | 0.6977 |
| 2 | -5.5280 | -6.4175 | -6.4175 | 0.8554 | 1.9330 | -0.4537 |
| 3 | -0.1391 | -6.4175 | -5.9413 | 0.3655 | 1.1730 | 1.1253 |
| 4 | 1.1747 | 0.8554 | 0.3655 | -3.4959 | 0.7435 | 0.4116 |
| 5 | 2.5311 | 1.9330 | 1.1730 | 0.7435 | -0.9285 | -0.7508 |
| 6 | 0.6977 | -0.4537 | 1.1253 | 0.4116 | -0.7508 | 1.4925 |
| 8% weight $SiO_2$ | | | | | | |
| *Cij* (GPa) | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 2.2389 | 4.5478 | 5.2813 | 0.2413 | 0.1288 | -1.8123 |
| 2 | 4.5478 | 1.1386 | 2.2619 | 0.2992 | 0.8973 | -3.0083 |
| 3 | 5.2813 | 2.2619 | -0.2744 | -0.3605 | 0.7388 | -2.6279 |
| 4 | 0.2413 | 0.2992 | -0.3605 | 3.9519 | 0.5022 | -1.5393 |
| 5 | 0.1288 | 0.8973 | 0.7388 | 0.5022 | 0.0647 | 0.7177 |
| 6 | -1.8123 | -3.0083 | -2.6279 | -1.5393 | 0.7177 | 0.9529 |
| 10% weight $SiO_2$ | | | | | | |
| *Cij* (GPa) | 1 | 2 | 3 | 4 | 5 | 6 |
| 1 | 48.7789 | 8.3751 | 10.5926 | 0.6053 | -0.5311 | 0.3190 |
| 2 | 8.3751 | 37.0461 | 9.7091 | 0.2639 | 0.1196 | 0.0847 |
| 3 | 10.5926 | 9.7091 | 55.1211 | 2.0672 | -1.2032 | 0.0838 |
| 4 | 0.6053 | 0.2639 | 2.0672 | 51.3748 | -0.3027 | -0.6237 |

| | | | | | | |
|---|---|---|---|---|---|---|
| 5 | -0.5311 | 0.1196 | -1.2032 | -0.3027 | 21.5979 | 0.6151 |
| 6 | 0.3190 | 0.0847 | 0.0838 | -0.6237 | 0.6151 | 27.1445 |

**Table 3.** The Compressibility, Bulk modulus and Shear modulus of epoxy/$SiO_2$ unit cell

| formula | | | Reuss | Voigt | Hill | Compressibility (1/TPa) |
|---|---|---|---|---|---|---|
| 6% weight $SiO_2$ | Bulk modulus (GPa) | | 0.0000 | -3.5617 | -1.7809 | -444.8762 |
| | Shear modulus (GPa) | | 0.0000 | -0.3065 | -0.1532 | |
| 8% weight $SiO_2$ | Bulk modulus (GPa) | | 7.0996 | 3.0317 | 5.0656 | 140.8531 |
| | Shear modulus (GPa) | | 0.0000 | 0.3947 | 0.1973 | |
| 10%weight $SiO_2$ | Bulk modulus (GPa) | | 21.3451 | 22.0333 | 21.6892 | 46.8491 |
| | Shear modulus (GPa) | | 23.492 | 27.5081 | 25.5004 | |

It can be seen from Table 1 that the value of C13, C55 and C56(6% weight $SiO_2$), C33 and C34(8% weight $SiO_2$ ),C15, C45 and C46(10% weight $SiO_2$ ) are close to zero, which indicates that the polymer model simulated by molecular dynamics is not extreme anisotropic material.

After the initial unit cell was prepared, 100ps of isothermal-isobaric ensemble referred to as NPT simulation at 1 atm with 1fs integration step of time, at room temperature was performed 298K.

By increasing the pressure, the system has been compressed for increase the density and NPT simulation just for once, the compressibility, bulk modulus and shear modulus of epoxy/$SiO_2$ unit cell were shown in Table 3. Curve of the cell density varies with time after simulation is shown in Figure 4, in this figure it can be noted that the density increased as the weight percent of $SiO_2$ increased at 5ps , its effective density can be increased by roughly 10% as compared to the EPON 862 matrix for 6% noano particles of $SiO_2$ weight percent.

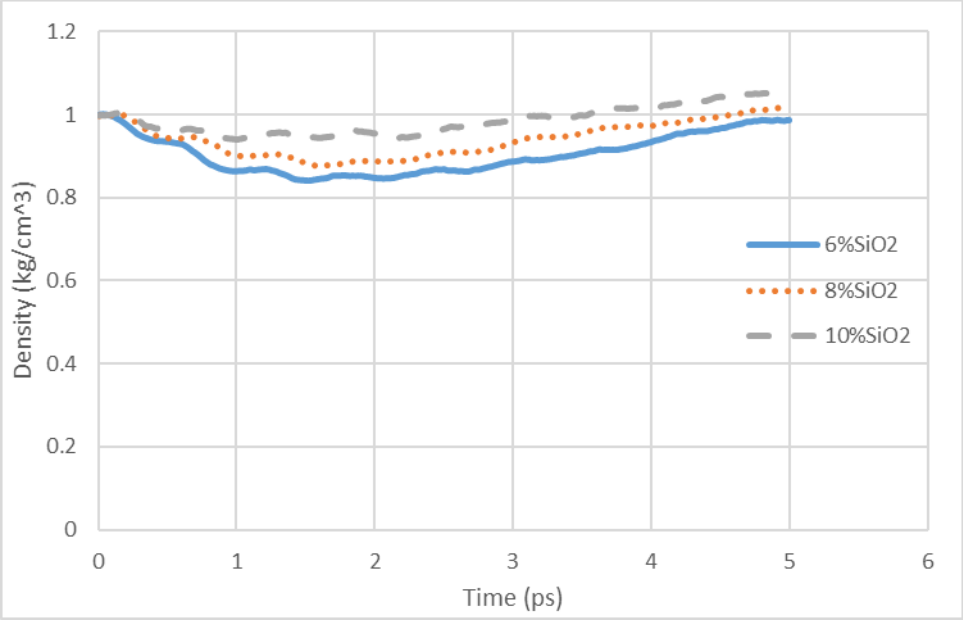



**Figure 4.** Forcite dynamic density

## 5. Conclusion

It is observed that the time reducing by using molecular dynamic simulation for studying the additives of $SiO_2$ particle to the epon 862 cross link TETA, due to the ability of accelery material studio program. As the weight percent increase from 6% to 10% $SiO_2$ the densities increase, bulk and shear modulus value is maximum in 10%addition.

## References

[1] Suyoung Y, Seunghwa Y., and Maenghyo C 2009, Multi-scale modeling of cross-linked epoxy nanocomposites, *J. Polymer*. **50**: 945-952.
[2] Komuves F, Kelkar A D, Mohan R, and Kelkar V A 2011, Prediction of Mechanical Properties of EPON 862 (DGEBF) cross-linked with Curing Agent W (DETDA) and SWCNT using MD Simulations, Structural Dynamics and Materials Conference 19th, Denver, Colorado, 4 - 7.
[3] Rai A K , Amit Porwal A and Mishra S B 2013, Investigation of mechanical properties of epoxy EPON 862 cured with TETA by molecular dynamics, S-JPSET : ISSN : 2229-7111, Vol. **4**, Issue 2.
[4] Kim B, ChoI J ,Yu S, Yang S and Cho M 2013, Effect of different crosslink densities on the thermomechanical properties of polymer nanocomposites, *Jeju, Korea J. Advanced in structure engineering and mechanics,* 8-12.
[5] Arab B, Shokuhfar A 2013, Molecular Dynamics simulation of cross-linked epoxy polymers: the effect of force field on the estimation of properties, *J. nano and electronic physics*. **5** No 1.
[6] Bharadwaja S 2012, Molecular dynamics simulations of Si binding and diffusion on the native and thermal silicon oxide surfaces molecular dynamics simulations of Si Binding and diffusion on native and Thermal Silicon Oxide Surfaces, theses(Msc).
[7] Mo Y, Zhang H and Xu J 2014, Molecular dynamic simulation of the mechanical properties of PI/SiO2 nanocomposite based on materials studio *J. chemical and pharmaceutical research*, **6(**6):1534-1539.
[8] Leach A R 1997, Molecular modelling: principles and applications, Addison Wesley Publishing Company.