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Molecular dynamic simulation of the density and mechanical properties of polyvinyl chloride(PVC)/high density polyethylene (HDPE) composites based on materials studio

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Molecular dynamic simulation of the density and mechanical properties of polyvinyl chloride(PVC)/ high density polyethylene (HDPE) composites based on materials studio

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Abstract— Initial unit cell models of polyvinyl chloride(PVC)/ high dnsity polyethylene (HDPE) composites and pure polyvinyl chloride were built using materials Studio, the stiffness matrix and mechanical parameters of the unit cells were achieved by molecular dynamic optimizations and calculations. Finally, the mechanical properties of pure PVC and the PVC/HDPE composites were compared. The result shows that the mechanical properties of PVC can be remarkably reinforced by being filled with HDPE, where the addition of 9.5%high density poly ethylene (HDPE) to poly vinyl chloride (PVC) the mechanical properties improved and the density degreases slightly.

Keywords—PVC, Material Studio, HDPE, molecular dynamics, mechanical properties

1. Introduction

The properties of polymer materials can be predicted by molecular dynamics simulations tools especially in the design of new materials in particular applications.

In this paper, the molecular dynamics method was used to calculate the physical and mechanical properties of polyvinyl chloride (PVC) / High Density Polyethylene (HDPE). Calculation of the properties was performed using the constant- strain (static) approach. A simulations were carried by used force fields; COMPASS which can be reliably used for simulation of polymers and determination of their properties [1].

2. Molecular Structure

A. polyvinyl chloride (PVC)

First, chains of length 80 units was generated using build homopolymers module from library in material studio, in order to generated the molecular structures of of polyvinyl chloride (PVC) is represented as shown in Figure. 1.

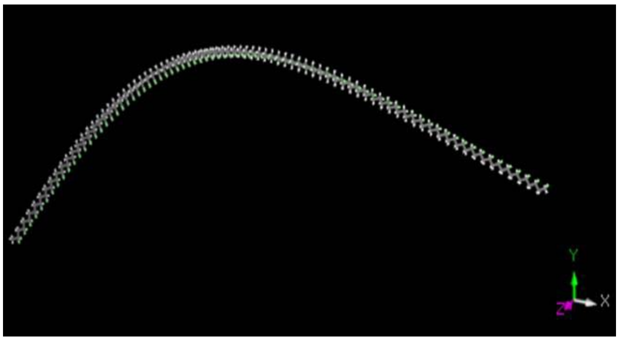

Figure. 1 . Molecular structures of polyvinyl chloride (PVC)

B. High density polyethylene (HDPE)

High density polyethylene (HDPE) was generated using ethylene from define fragment browsers, then high density polyethylene build by select head and tall for 10 units length ;see shown in Figure. 2 .

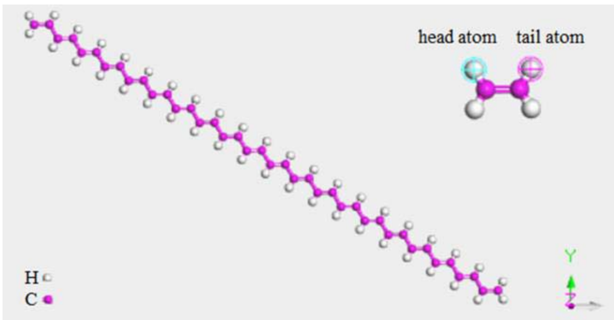

Figure 2 . High Density Polyethylene (HDPE)

3. Simulation Details

Molecular dynamics simulations are performed by using materials stuidio v.7.0 software packet copy right 2013, Accelrys Inc., After, homopolymers of PVC and HDPE built, models are constructed from 100% weight of PVC with the unit cell as cubic lenght (A^o) 20.3×20.3×20.3, and 90.5% PVC added to 9.5% HDPE with the unit cell as cubic lenght (A^o) 20.9×20.9×20.9m see Figure. 3 and Figure. 4. To avoid errors during simulation geometry optimization were calculated in each model using forcite calculation.100 repeated units are involved. Then 10 amorphous structures of the polymer are generated with periodic boundary conditions.

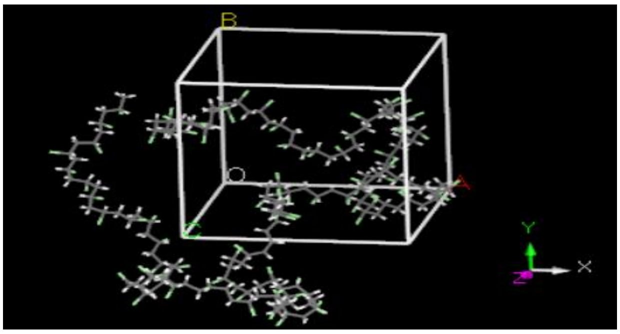

Figure 3 . Unit cell of 100% weight of PVC

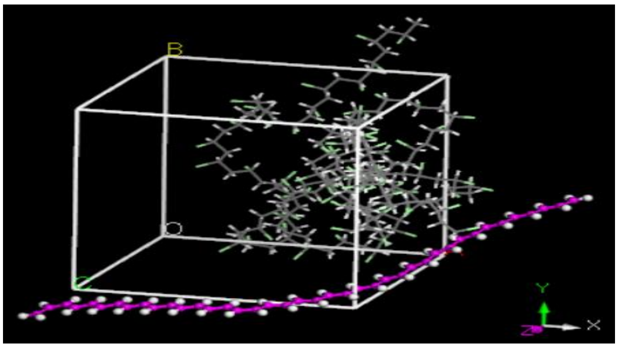

Figure. 4 .Unit cell of 90.5% PVC and 9.5% HDPE

4. Results and Discussion

The calculated of densities of the final structure in 5000 steps of NPT (constant number of atoms, volume and temperature) at 1.0 fs time step, 298 K. Density are plotted with respect to time as shown in Figure. 5. and Figure. 6.

The density of the PVC will increase steadily. A clear change in the slope of the curve of Figure. 6, as compared with Figure.5., This caused by the addition of HDPE, where the changing of densities are from 1.26 g/cm^3 to 1.13g/cm^3.

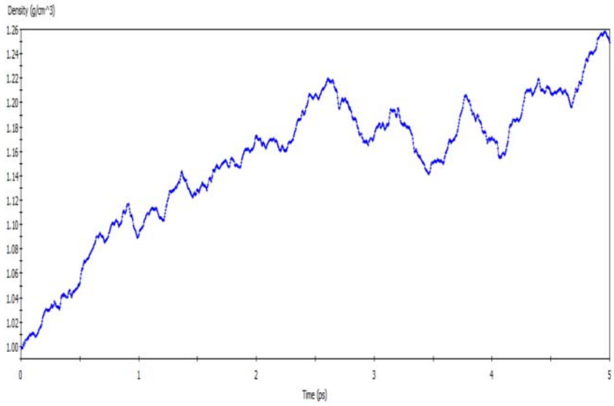

Figure. 5 . Density of 100% weight of PVC

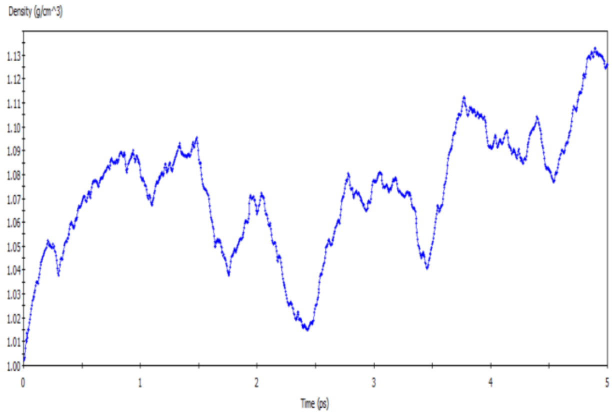

Figure. 6 . Density of 90.5% PVC and 9.5% HDPE

After open the calculation dialog from Select modules of forcite calculation,(dynamics), the results of this include the files of the density, cell size curves , energy, convergence[2], it can be see that from Figureures from 7 to 8, the variation of the cell length decrease from 20.3 to 18 in pure PVC and decrease from 20.9 to 20.1 in 90.5% PVC 9.5%HDPE. But the angle of cubic cell remain without change during periodic of time in both pure PVC and additions of 9.5%as in Figureures 9 and 10.

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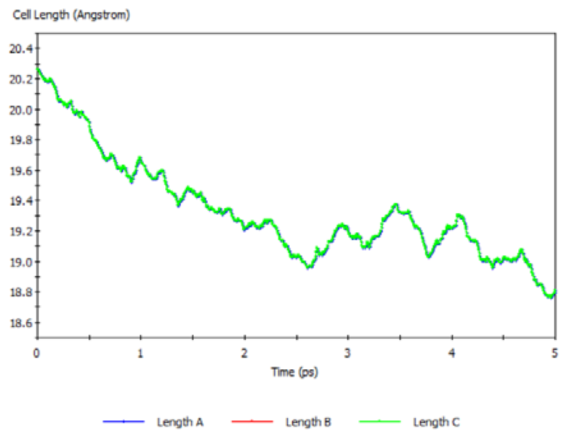

Figure. 7 . Forcite dynamics cell lenghts of 100% PVC

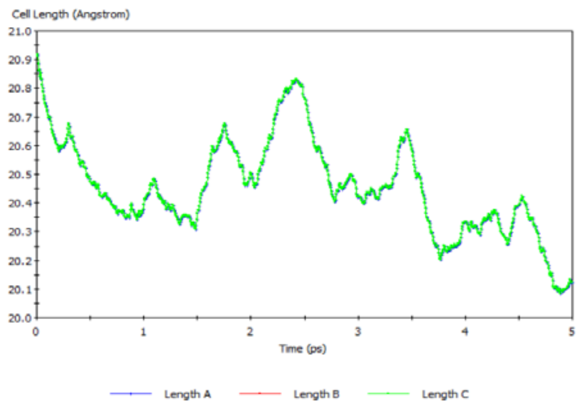

Figure. 8 . Forcite dynamics cell lenghts of 90.5% PVC and 9.5% HDPE

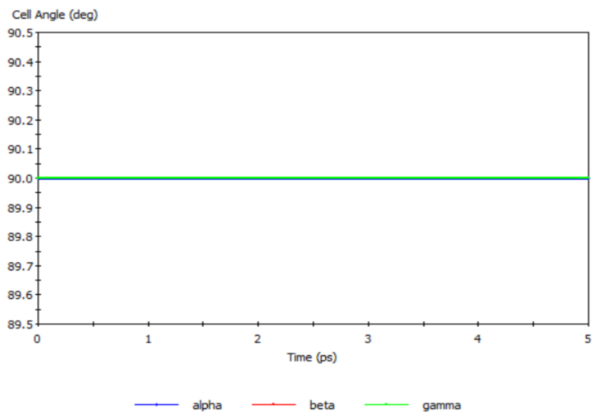

Figure. 9 . Forcite dynamics cell angles of 100% PVC

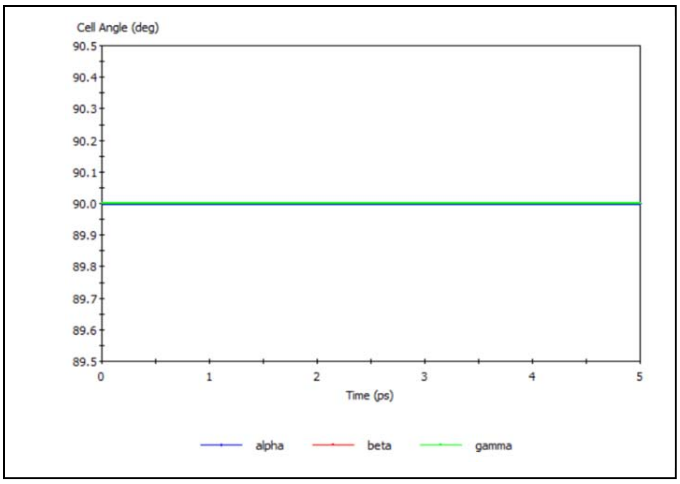

Figure. 10 . Forcite dynamics cell angles of 90.5% PVC and 9.5% HDPE

For isotropic material, the Young" modulus can be determinations by using equations formula dependents on elastic stiffness which are results from simulations[3].

For 100% weight of PVC elastic stiffness constants Cij (GPa), Stress-i = Cij*Strain-j.

-2.1874	-1.2352	-0.3194	0.3708	-0.2158	0.6598
-1.2352	0.5144	0.1412	-0.1005	-0.3275	0.5575
-0.3194	0.1412	0.3641	0.2433	-0.5772	-0.1763
0.3708	-0.1005	0.2433	1.1094	0.3230	-0.1248
-0.2158	-0.3275	-0.5772	0.3230	0.0858	0.3232
0.6598	0.5575	-0.1763	-0.1248	0.3232	-1.2373

For 100% weight of PVC elastic compliance constants Sij (1/TPa), Strain-i = Sij*Stress-j.

-387.8699	-435.4559	199.5971	-81.0080	304.8751	-343.6753
-435.4559	904.8677	-51.7168	150.5860	409.2488	274.5878
199.5971	-51.7168	-261.0998	444.3410	-1718.9101	-373.4311
-81.0080	150.5860	444.3410	668.7612	626.2728	57.4505
304.8751	409.2488	-1718.9101	626.2728	-972.7572	274.6821
-343.6753	274.5878	-373.4311	57.4505	274.6821	-748.5702

For 90.5% PVC and 9.5% HDPE elastic stiffness constants Cij (GPa), Stress-i = Cij*Strain-j.

2.3200	2.4022	0.4931	0.7934	-0.5722	0.5690
2.4022	4.7830	0.3025	0.7117	-0.3430	0.3843
0.4931	0.3025	2.1985	0.9221	0.3006	-0.6075
0.7934	0.7117	0.9221	0.7554	-0.2771	0.5477
-0.5722	-0.3430	0.3006	-0.2771	0.1884	-0.0109
0.5690	0.3843	-0.6075	0.5477	-0.0109	-0.0076

For 90.5% PVC and 9.5% HDPE elastic compliance constants Sij (1/TPa), Strain-i = Sij*Stress-j.

1994.9908	-699.8189	137.1232	-1363.2466	2618.9470	993.5707
-699.8189	493.3128	-42.3299	314.6576	-717.5694	-352.9569
137.1232	-42.3299	206.1303	110.7387	140.3110	-572.3721
-1363.2466	314.6576	110.7387	1288.9541	-1819.3347	507.1800
2618.9470	-717.5694	140.3110	-1819.3347	9293.5285	4112.8794
993.5707	-352.9569	-572.3721	507.1800	4112.8794	1364.0368

It was observed from the above there are increasing in elastic stiffness of added HDPE as compared without addions to PVC.

Table1. value of young modulus and poisson ratios

Young Modulus (GPa)		Poisson Ratios			
For 100% PVC					
X =	-2.5782	Exy =	-1.1227	Exz =	0.5146
Y =	1.1051	Eyx =	0.4812	Eyz =	0.0572
Z =	-3.8300	Ezx =	0.7644	Ezy =	-0.1981
For 90.5% PVC and 9.5% HDPE					
X =	3.8225	Exy =	-0.2884	Exz =	-0.9128
Y =	5.3773	Eyx =	-0.4057	Eyz =	0.7000
Z =	2.3662	Ezx =	-0.5650	Ezy =	0.3080

Young‟s modulus of 90.5% PVC and 9.5% HDPE calculated was compared with the young‟s modulus of 100%. As shown in table I., which shows that Young‟s modulus variation of 90.5% PVC and 9.5% HDPE higher than 100% PVC .

5. CONCLUSIONS

molecular dynamic simulation used in this work,in order to reduce cost which are resulted from experimental.

Molecular dynamic simulation used to predict the mechanical properties,

The addition of 9.5%high density poly ethylene (HDPE) to poly vinyl chloride (PVC) improved the mechanical properties and degreases density slightly, so it is changing other relater properties which are needed in some importance applicatios.

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