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Investigation of mechanical properties of BaTiO3/PVDF nanocomposites: A molecular dynamic simulation

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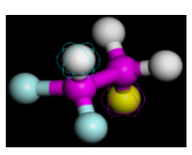
INTRODUCTION

Poly (vinylidene difluoride) (PVDF) is a semi-crystalline polymer that is widely used in fields where chemical resistance, abrasion and thermal stability are required. PVDF has been widely investigated since it exhibits many remarkable properties in terms of **good mechanical properties**, **resistance to chemicals**, **high dielectric permittivity** and **unique pyroelectric** and **piezoelectric properties** in practical applications. But, pure PVDF cannot meet the requirements of mechanics, thermology and oxidation resistance completely. **Incorporation of ceramic particles** with high dielectric permittivity into the polymeric matrices is considered to be one of the most common and promising strategies, which takes the advantages of colossal permittivity of ceramic particles and good dielectric strength of polymers. Poly (vinylidene fluoride) (PVDF), a ferroelectric polymer with relatively high dielectric permittivity, was widely investigated in the formation of the dielectric composites with addition of ferroelectric ceramic fillers, such as $BaTiO_3$, and $Ba_{0.6}Sr_{0.4}TiO_3$.

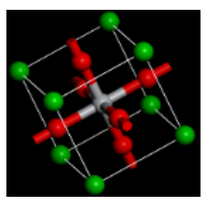
OBJECTIVE

Molecular dynamics (MD) simulation was performed to study the mechanical properties of poly(vinylidene fluoride)- (PVDF) based composites with different contents of barium titanate BTO by using Material Studio (MS) software.

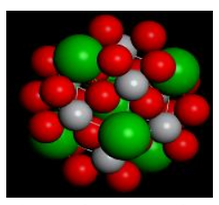
MOLECULAR MODELS



PVDF monomer



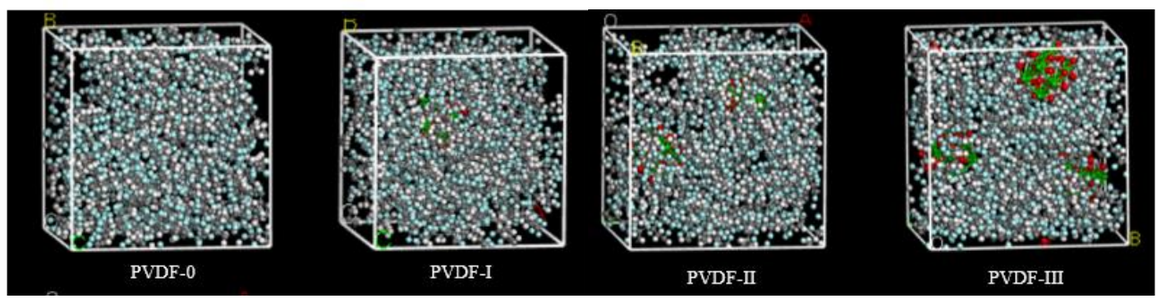
Crystal structure of BTO



BTO spherical particles

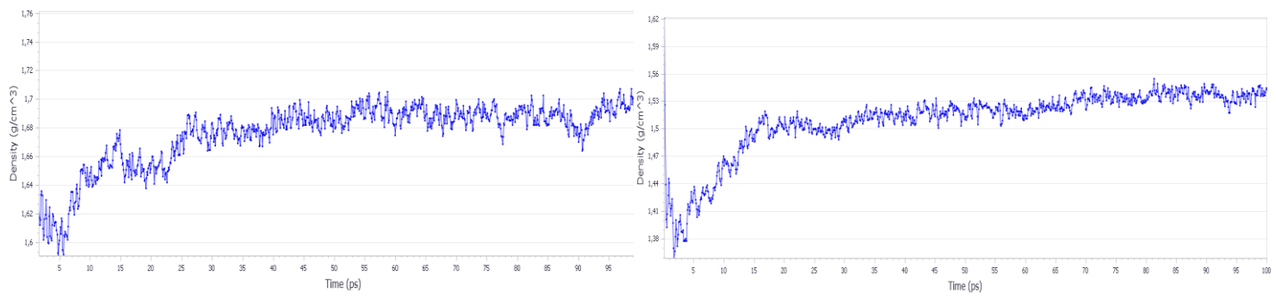
MOLECULAR DYNAMICS SIMULATIONS

- All simulations were performed using the UNIVERSAL force field, is the excellent general purpose forcefield. The parameters are generated from a set of rules based on element, hybridization and connectivity.
- The cubic unit cells of mixtures of PVDF and BTO were built as five PVDF macromolecular chains and different amounts of BTO particles: 0, 1, 2 and 3.



- After constructing the initial models, the geometric structure was **optimized** by the Smart algorithm
- To obtain the true density of material, the Molecular Dynamics Simulation is necessary. The cell density gradually increases under external pressure, and the system can be further compressed by increasing the pressure via **NPT simulation**.
- When the density was close to the experimental value, enough time of isothermal ensemble referred to as **NVT** ensemble simulation was performed to balance the system.

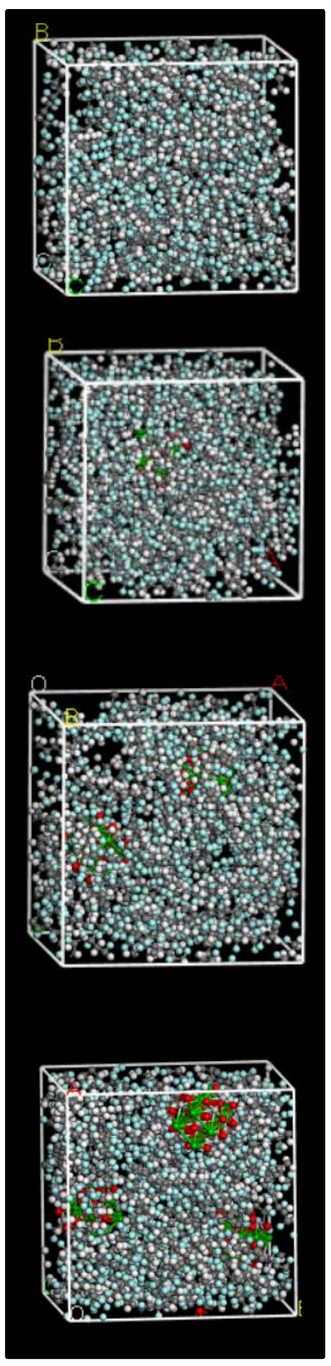
(a) **(b)**



Cell density with respect to time under 0.15GPa of the PVDF-0 (a) and PVDF-III (b)

RESULTS & DISCUSSION

- The elastic stiffness matrix of four systems obtained from the MD simulations which is obtained by the Forcite calculation available in the module tool of Material Studio software to calculate its mechanical properties.



Cij(GPa)	1	2	3	4	5	6
1	2.34	1.21	1.15	0.04	0.01	0.03
2	1.21	2.31	1.11	0.00	0.00	0.04
3	1.15	1.11	1.86	-0.06	-0.02	-0.02
4	0.04	0.00	-0.06	0.48	-0.03	0.02
5	0.01	0.00	-0.02	-0.03	0.62	0.02
6	0.03	0.04	-0.02	0.02	0.02	0.79

Cij(GPa)	1	2	3	4	5	6
1	3.10	1.63	1.63	0.20	0.01	0.17
2	1.63	3.56	1.48	0.04	0.04	0.00
3	1.63	1.48	3.19	0.11	-0.10	0.06
4	0.20	0.04	0.11	0.77	0.07	0.01
5	0.01	0.04	-0.10	0.07	0.93	0.07
6	-0.17	-0.01	0.06	0.01	0.07	1.06

Cij(GPa)	1	2	3	4	5	6
1	4.65	2.67	2.77	-0.00	-0.18	0.03
2	2.67	4.58	2.47	-0.02	-0.02	0.05
3	2.77	2.47	3.63	0.07	-0.02	0.20
4	-0.00	-0.02	0.07	0.84	0.04	-0.06
5	-0.18	-0.02	-0.02	0.04	1.13	-0.02
6	0.03	0.05	0.20	-0.06	-0.02	1.15

Cij(GPa)	1	2	3	4	5	6
1	3.90	1.81	1.87	0.01	-0.39	0.08
2	1.81	2.98	1.52	0.05	0.13	0.04
3	1.87	1.52	2.85	0.10	-0.63	0.04
4	0.01	0.05	0.10	0.62	0.05	-0.06
5	-0.39	0.13	-0.63	0.05	1.24	0.01
6	0.08	0.04	0.04	-0.06	0.01	1.11

- The polymer model simulated by molecular dynamics is not extreme anisotropic material.
- The model is close to the isotropic material. So, it can be assumed that the material is isotropic.

- For the composite PVDF-I with a nanoparticle content of 7.57 wt%, the Young's modulus, bulk modulus, and shear modulus all increase markedly compared to pure PVDF.

	Young's Modulus (E)	Bulk Modulus (K)	Shear Modulus(G)
Pure PVDF	2.34	2.51	0.67
PVDF-I	4.65	4.95	1.32
PVDF-II	3.90	4.00	1.12
PVDF-III	3.10	3.20	0.90

- However, as the nanoparticle content increases to 14.07 wt% (PVDF-II) and 19.72 wt% (PVDF-III), a gradual decrease in all moduli is observed.

CONCLUSION

- Molecular modeling of BTO/PVDF nanocomposites has developed to determine the elastic constants such as Young's modulus, bulk modulus, shear modulus.
- In this study, the MD simulation approach with UNIVERSAL force-field has been effectively applied to simulate the PVDF nanocomposites with different wt% of BTO.
- The constant strain approach has been used to calculate the mechanical properties of nanocomposites.