INTERACTION OF GRAPHENE AND POLYCAPROLACTONE AT ATOMIC LEVEL

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ABSTRACT

Polycaprolactone (PCL) is a material widely used in regenerative medicine because of biocompatibility, biodegradability, and low toxicity. Applications of PCL are mainly focused on tissue engineering, wound healing, drug encapsulation and delivery etc. PCL scaffolds have been used for stem cell differentiation into various cellular lineages. However, the hydrophobicity of PCL scaffolds possess some limitation to cellular attachment. Graphene which is a single sheet of sp2 hybridized carbon atoms can enhance cellular attachment by establishing π-π interaction. Here we investigate the interaction of PCL and graphene by molecular dynamics simulation and hence fabrication of PCL scaffolds with graphene nano-inclusions for neuronal differentiation. Correlated conformational and energetic analysis are implemented. During 10ns simulation, randomly assigned PCL chains adsorbed onto the surface of graphene and the size of PCL also tended to fit graphene sheet. Wrapping phenomenon was detected after 10ns interaction. The dominant force is Van der Waal's force and hydrophobic interaction.

INTRODUCTION

The PCL-G scaffolds were fabricated by the process of electrospinning. The viscoelastic polymer solution of PCL dispersed with graphene was stretched under electric field, so as to collect the fibers on a collector oppositely charged. To deepen our understanding of interaction of PCL with graphene at atomic level we utilized molecular dynamics to analyze the conformational and energy changes when the two molecules are brought closer.

METHODS

5 nm×5 nm armchair graphene sheet was generated by Nanotube builder. PCL chains of 16 caprolactone monomers were prepared in ChemBioDraw Ultra13.0. Ten PCL chains were randomly placed on top of graphene, the distance between the center of PCL and graphene is set to 10 nm (Figure 1). Graphene and PCL system is solvated into 17Å×17Å×41Å TIP3P water box and the whole system was neutralized by 0.15mol/L NaCl. System experienced 5, 000 steps minimization and followed 50 million steps simulation (100ns, 500steps/ps) with Charmm 36 forcefield.

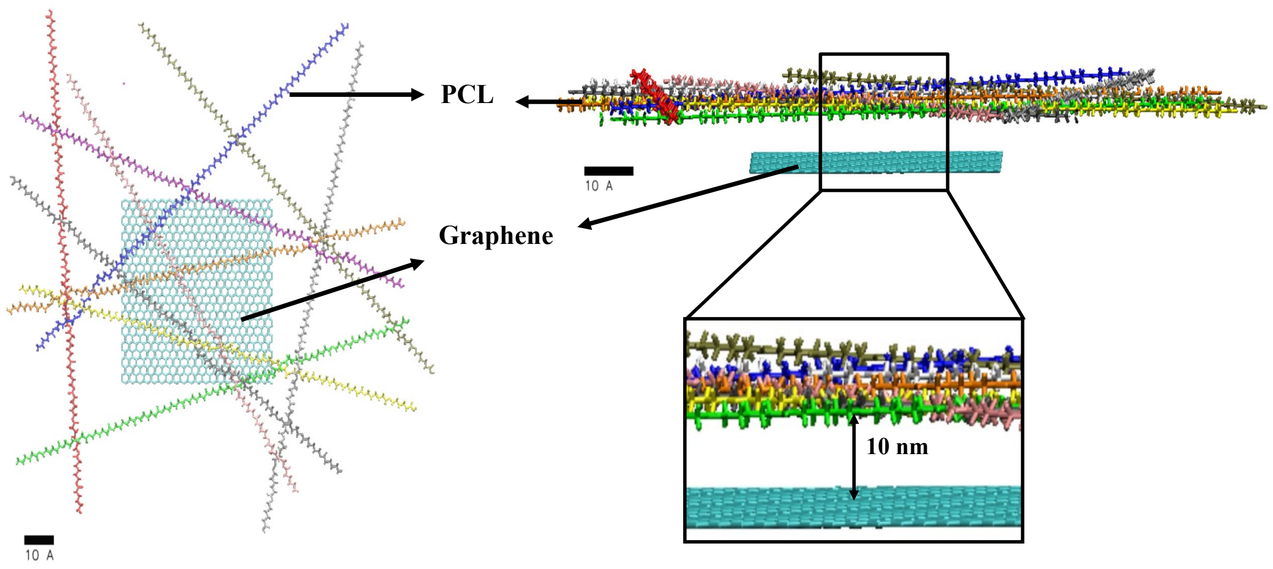

Figure 1. Left: Top view of graphene-PCL scaffold**. Upper right:** Side view of graphene-PCL scaffold. **Bottom right:** The distance between graphene and PCL is 10 nm.

CONCLUSION

In the first 10ns of simulation, the PCL chains stabilized on the surface of graphene, the wrapping phenomenon of PCL chains was detected at the end of interaction. Center of mass distance between graphene and PCL also decreased, indicating the attraction effect within the system. This result also consistent with Van der Waal's energy, which remained negative throughout the simulation, which means strong attractive interaction exists between PCL and graphene. In addition, hydrophobic interaction also contributed to such process.

RESULTS

Microstructure of PCL-G scaffold shown in Figure2. After 10 ns simulation, conformational and energetic analysis (Figure 3) are implemented by user-defined tcl scripts. Data are plotted by GraphPad Prism 7.

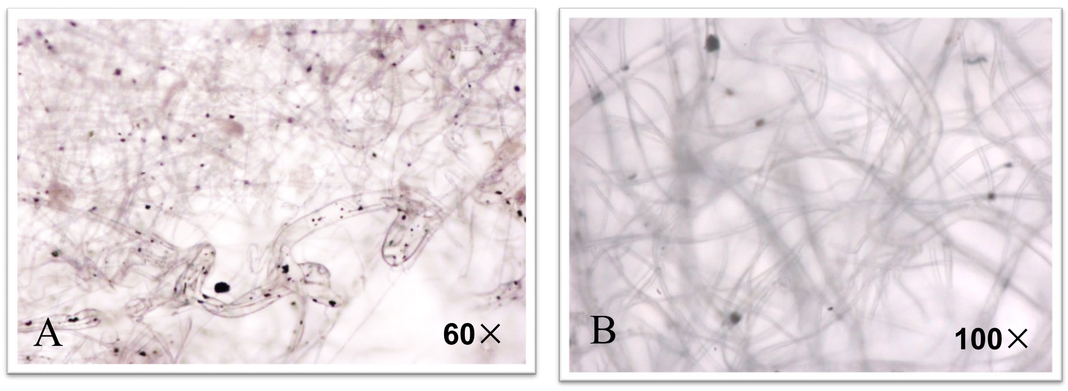

Figure 2. Structure of PCL-G under light microscope

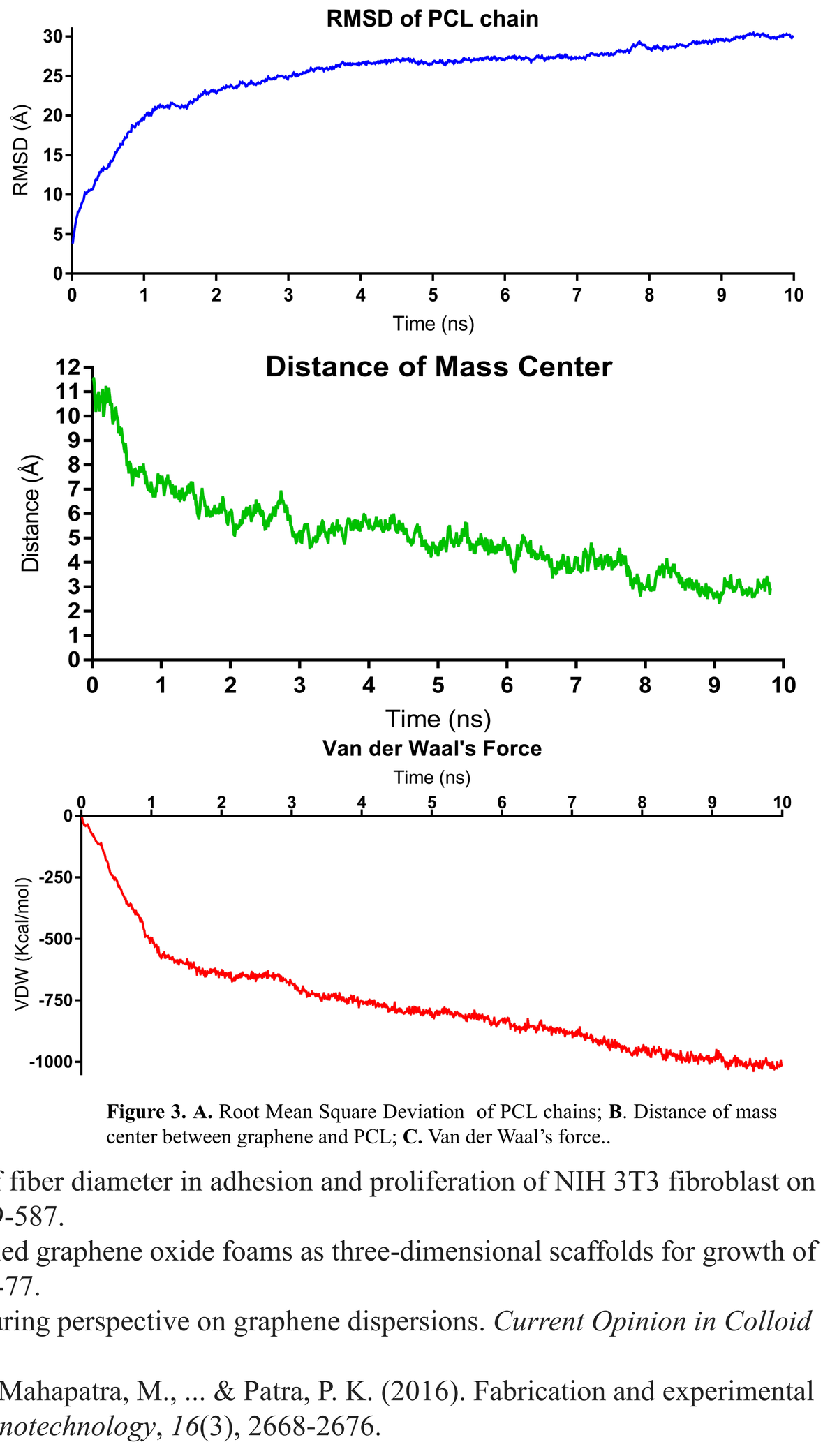

Figure 3. A. Root Mean Square Deviation of PCL chains; **B**. Distance of mass center between graphene and PCL; **C.** Van der Waal's force..

REFERENCES

1. Chen, M., Patra, P. K., Warner, S. B., & Bhowmick, S. (2007). Role of fiber diameter in adhesion and proliferation of NIH 3T3 fibroblast on electrospun polycaprolactone scaffolds. *Tissue engineering*, *13*(3), 579-587.
2. Akhavan, O., Ghaderi, E., Shirazian, S. A., & Rahighi, R. (2016). Rolled graphene oxide foams as three-dimensional scaffolds for growth of neural fibers using electrical stimulation of stem cells. *Carbon*, *97*, 71-77.
3. Johnson, D. W., Dobson, B. P., & Coleman, K. S. (2015). A manufacturing perspective on graphene dispersions. *Current Opinion in Colloid & Interface Science*, *20*(5-6), 367-382.
4. Aphale, A. N., Mahakalkar, K., Macwan, I. G., Mukerji, I., Cox, P. J., Mahapatra, M., ... & Patra, P. K. (2016). Fabrication and experimental analysis of axially oriented nanofibers. *Journal of nanoscience and nanotechnology*, *16*(3), 2668-2676.