

Length Dependent Interactions of Carbon Nanotubes and Surfactant Protein B



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Abstract

Molecule dynamics (MD) simulation is a powerful computational tool to study the interaction between two or more molecules. In this poster, we present the interaction of carbon nanotubes (CNT) with surfactant protein B (SPB). SPB is a member of pulmonary surfactant protein family, which contributes to maintain alveolar surface tension. The lack of pulmonary surface tension will lead to collapse of alveoli in infants. This is the leading cause of infant respiratory distress syndrome (IRDS). To develop CNT based biosensor, study of these interactions between sensor material (CNT) and protein (SPB) at atomic level is very important. In practical situation, many protein molecules may surround the sensing element CNT. In this case, protein adsorption on CNT is influenced by CNT-proteins and protein-protein interactions. In addition, different lengths of CNTs also affect the rate of protein adsorption on CNT surface. Results show, as the length of CNT increases also increasing the specific surface area we see greater protein adsorption rate. All protein molecules experience different degrees of conformation change to achieve their stable state on CNT surface.

Introduction

We would like to develop a carbon nanotube-based biosensor to detect the level of pulmonary surfactant protein family in amniotic fluid. The very first thing is that we need to know the interaction between carbon nanotube and proteins. Here we choose surfactant protein B (SPB) as one sample for studying. SPB is a member of pulmonary surfactant protein family, which contribute to the maintain alveolar surface tension. Additionally, the length of CNT is also a factor that affects the interaction between these two things. Different length of CNT contributes to different behavior of SPB.

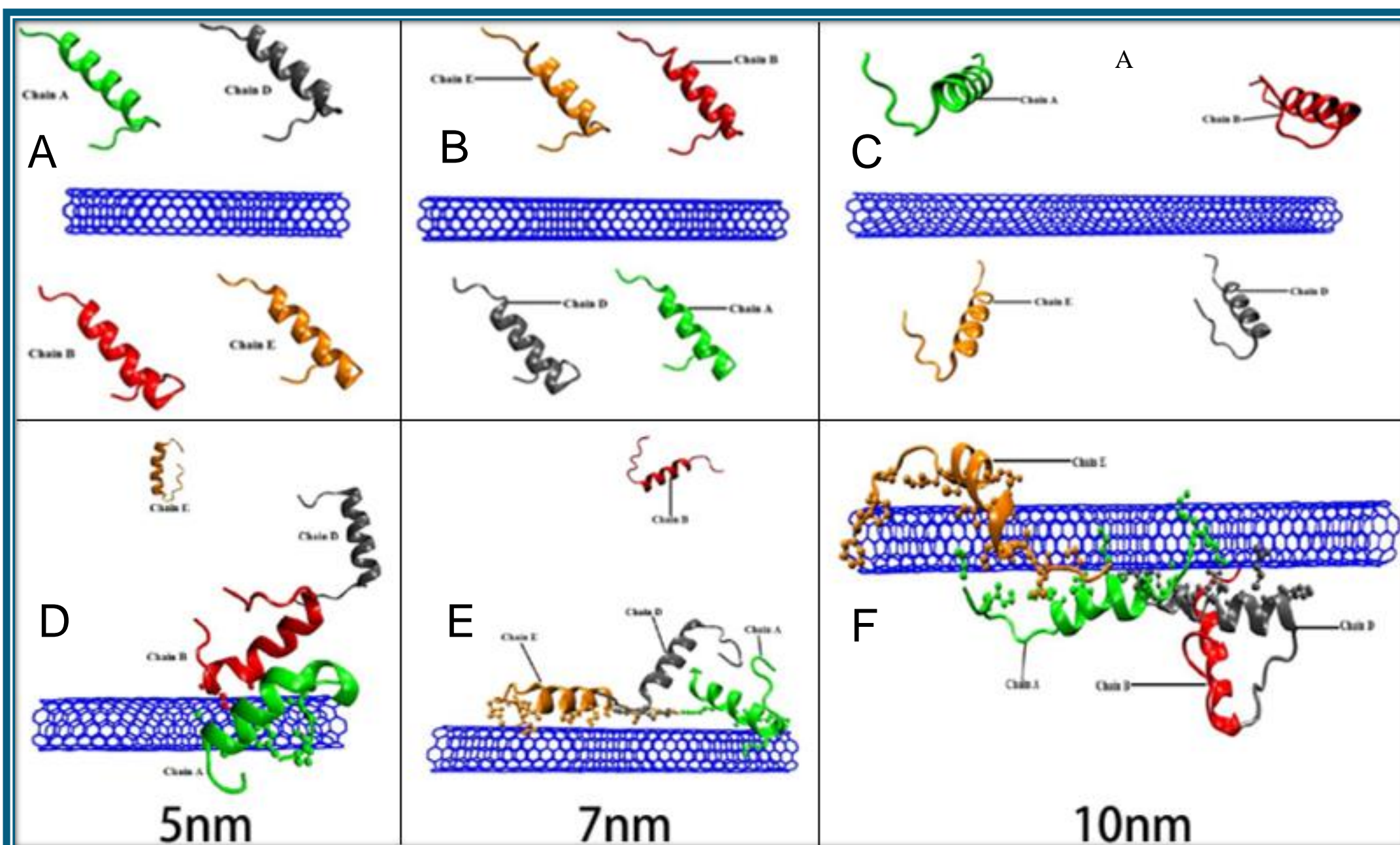


Figure 1A, B, C: Initial position of SPB with 5nm, 7nm and 10nm CNT
Figure 1D, E, F: Final position of SPB with 5nm, 7nm and 10nm CNT

Methods

We got SPB protein file from protein data bank (PDB) and use carbon nanostructure builder in VMD to generate 3 different lengths of CNTs (5nm, 7nm and 10nm), which are armchair nanotubes with chiral vectors of (6,6). To simulate the real natural situation, we put 4 SPBs sounded around one CNT. For identifying, we named them chain A, B, D and E. Distance between the center of SPB and CNT was 25 Å and the distances of SPBs that at the same side of CNT are 34.05Å for 5nm CNT, 33.48Å for 7nm CNT and 63.10nm for 10nm CNT. 5nm and 7nm systems underwent 100ns computation, 10nm system underwent 120ns computation. We applied CHARMM27 force field parameter to NAMD for molecular dynamics simulation.

Results

5nm CNT: After 100ns simulation, only 2 chains, chain A and chain B adsorbed onto the CNT surface. The value of RMSD (root mean square deviation) of chain A, chain B and chain E were similar.

7nm CNT: Compared to 5nm CNT, the number of adsorbed SPB increased, 3 chains went to the surface of CNT, chain A, chain D and chain E. Chain A showed the minimum RMSD value while chain E showed the maximum RMSD value.

10nm CNT: After 120ns computation, all 4 chains were adsorbed onto CNT surface, chain D showed the minimum RMSD value. Additionally, the interaction between proteins was founded.

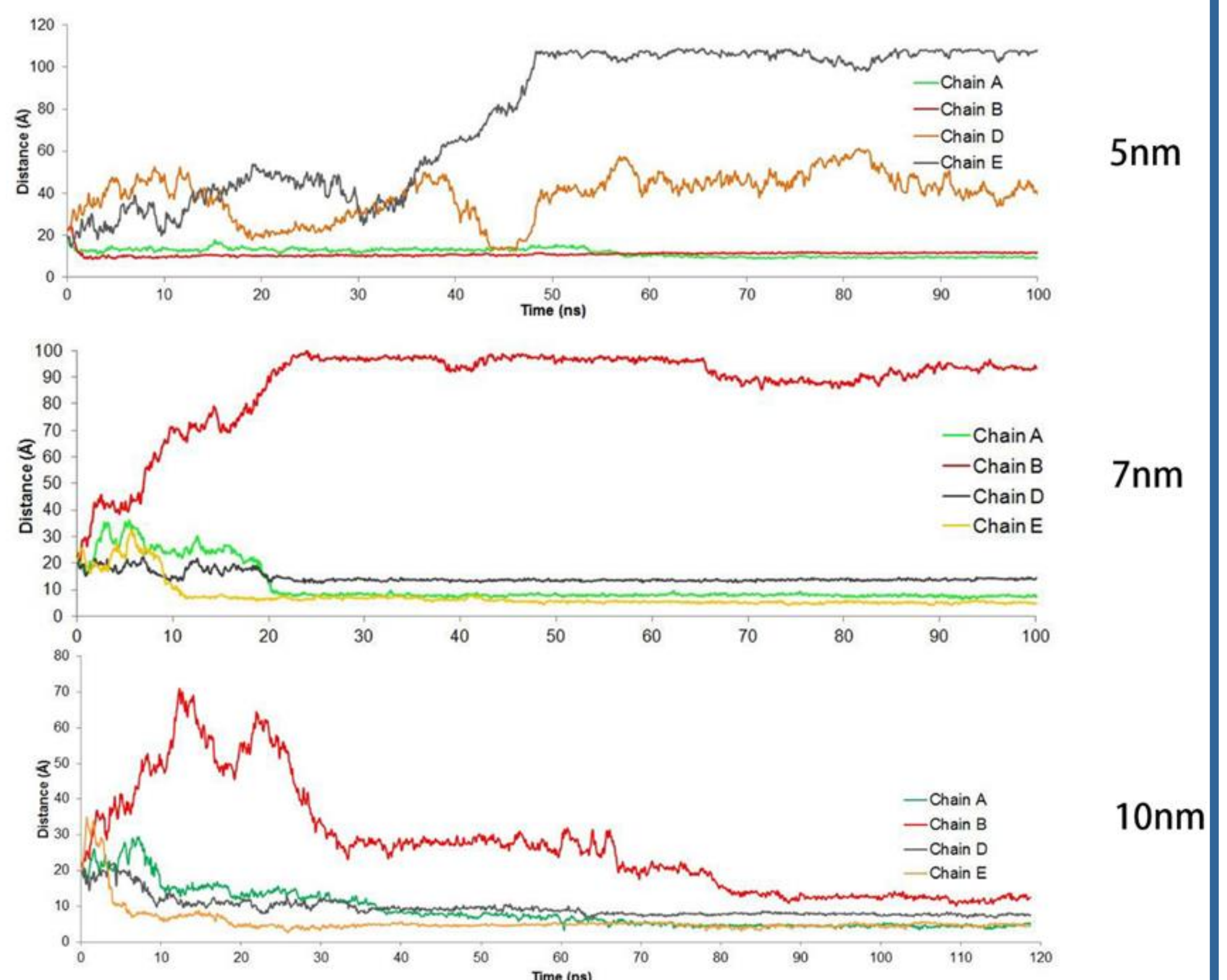


Figure 2: Distance between centers of protein molecules to 5nm, 7nm and 10nm carbon nanotubes for 100 ns. Four molecules of SP-B are named as Chain A, B, D and E. Results show the longer carbon nanotube possesses the ability to absorb more SPB molecules.

Conclusions and discussion

The number of adsorbed protein increases when extended CNT length. The longer the carbon nanotube, the more proteins can be adsorbed, this can be observed from Figure2. When multiple protein molecules interact with CNT surface then the adsorption of protein atoms on CNT surface is influenced by protein-CNT and protein-protein interactions. When protein-protein interaction occurs in this case the repulsive type of force is more dominant that is the reason in case of 5nm and 7nm protein molecules move away from the surface of CNT. In case of 10nm the protein-CNT interaction forces are greater than protein-protein interaction therefore, we observe complete protein adsorption.

References

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