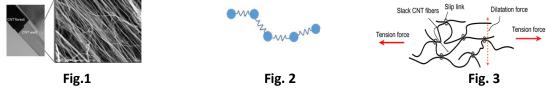
# Simulation of several CNT based macrostructures using Slip-Link model and Discrete Element Method

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### Introduction

The CNT macrostructures including membranes start by forming web on which CNT fibers are oriented along the web axis, some of them are parallel and others are poorly aligned or coiled [1]. Since the CNT web impacts on the properties of derived macrostructures, the simulation of CNT membranes attracted significant attentions [2]. The scanning electron microscopy analysis of CNT webs showed that CNT fibers entangle together (**Fig. 1**). This entanglement is a key factor for the formation of CNT macrostructures because it allows the array of parallel fibers to unfold continuously into CNT networks.



#### Aims

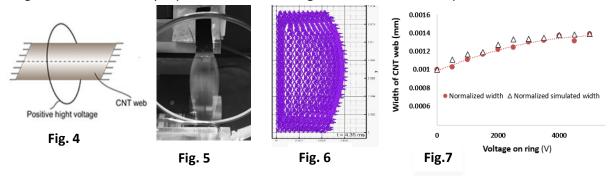
The work focuses on modelling the interconnection between CNT fibers within membranes and also other macro-structures and then analyzing mechanical properties of them.

### Methods

The entanglement of CNT fibers, as a chain of dumbbells (Fig. 2), can be regarded as networks made of fibers' entanglement junctions (Fig. 3), which impact on the properties of derived CNT macrostructures. Thus, the entanglement of CNT fibers is modelled using the dual slip-link theory [3]. The linkage can be destroyed if fibers slide off the slip links. This model corresponds to the formation of a random network of CNT fibers with non-uniform tension pulled out of a CNT forest. The simulation of the deformation of CNT membrane by load are developed using the Discrete Element Method (DEM)

## **Results & Discussion**

The present method was applied to analyze the deformation of a CNT membrane undergone an electrical field as shown in **Figs. 4&5**. The simulating results by the present method (**Fig. 6**) are in good agreement with ones by experiment as show in **Fig. 7**. More details will be presented in the conference.



## Conclusion

The work reports for the first time the simulation of CNTs macro-structures using the combination of dual slip-link entanglement model and DEM. The present approach yields a new technique to predict several mechanical properties of CNT macrostructures including the tensile strength and the deformation by loads. Several initial results were successfully investigated by experiment. **References** 

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- 3. Doi M & Takimoto, J. (2003). Molecular modelling of entanglement, *Philos. Trans. A. Math. Phys. Eng. Sci.*, 361(1805), 641–652.