# Exciton Diffusion Properties in Carbon Nanotube Films

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Carbon nanotube (CNT) films have been introduced into organic photovoltaic devices as optical absorbers [1]. Illumination generates excitons inside CNT films, so it is important to understand exciton diffusion properties for the purpose of improving device efficiency. We studied exciton transfer in binary CNT systems in our previous papers [2,3] and now introduce our new numerical tool DECaNT (Diffusion of Excitons in Carbon NanoTubes) [4] that simulates exciton diffusion in complex CNT films with various morphologies.

The simulation tool can be divided into two parts: a virtual CNT-film generator and a Monte Carlo simulator. The CNT generator uses the Bullet Physics C++ library to generate a realistic three-dimensional model of the CNT mesh with desired parameters (the chirality and length of each individual tube, intertube spacing, whether tubes are aligned in parallel, whether tubes are bundled or not, and the presence and density of trapping sites that can dissociate excitons). The Monte Carlo simulator captures exciton diffusion through the virtual CNT film. The simulator records the displacement of every exciton inside the CNT film at each simulation step, and calculates the diffusion tensor from the long-time limit of the position–position correlation function. It can also record exciton lifetime and calculate the diffusion length in the presence of disorder.

In Fig. 1, we present the cross-plane correlation functions versus time for films of CNTs with two different chiralities [(4,2) and (6,1)] and three different morphologies for each chirality (parallel, single tubes randomly oriented, and bundled tubes with bundles randomly oriented). Aligning tubes helps with exciton diffusion, but the magnitude of this effect depends on tube chirality. In Fig. 2, we show how intertube spacing affects the diffusion rate. The diffusion rate decreases with increasing intertube distance for all morphologies, with the decay being fastest in the parallel and slowest in the bundled random morphology. At the conference, we will also discuss the role of disorder in exciton diffusion length and lifetime, as well as the effects of possible polydispersity (mixture of chiralities) in CNT films.

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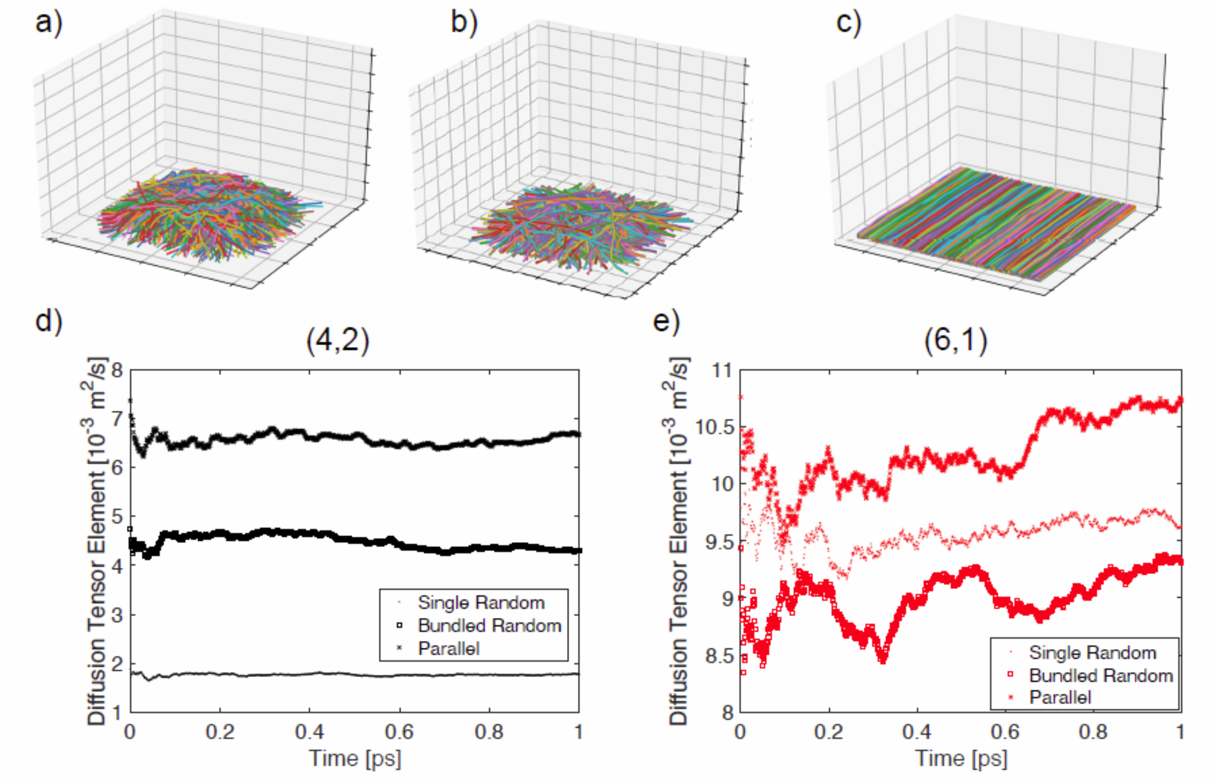

Fig. 1. Cross-plane position-position correlation function as a function of time (its long-time limit is the diffusion-tensor element) for two chiralities, (4,2) and (6,1) (panels (d) and (e), respectively) in the three film morphologies shown on top: (a) single random, (b) bundled random, and (c) parallel and each of the.

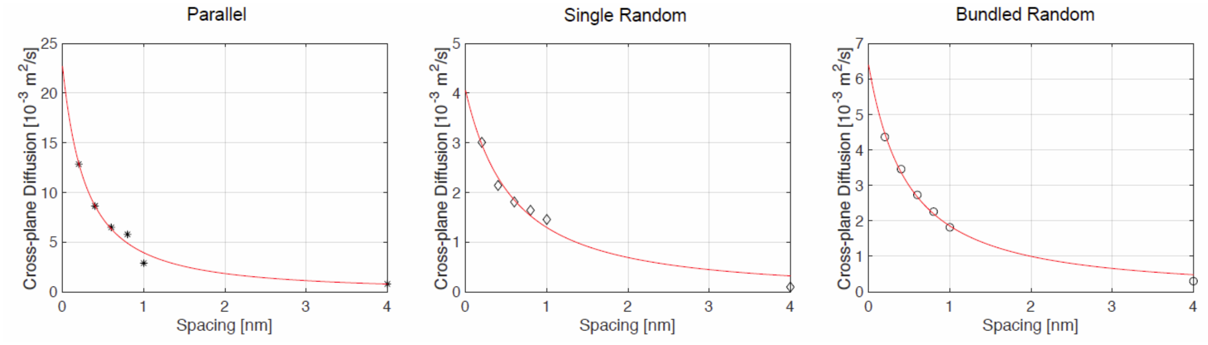

Fig. 2. Cross-plane diffusion-tensor element as a function of intertube wall-to-wall spacing. Diffusion decreases with increased spacing for all morphologies, but the rate of this decrease depends on morphology. The parallel morphology exhibits the quickest decrease, while the bundled random film exhibits the slowest. This is because CNTs with random orientation could be partially oriented in the cross-plane direction and CNTs within a bundle don't have added spacing, allowing for motion in the cross-plane direction within a given bundle. The red lines are fits according to $D(d)=D(0)/(d+d_0)^n$ , where d is the intertube spacing (horizontal axis in the graphs above), $d_0$ plays the role of an effective tube diameter and is dependent on morphology, and $n \approx 2$ [4].