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Brownian Dynamics Simulations of Single-Wall Carbon Nanotube (SWNT) Separation by Type using Dielectrophoresis MANUEL J. MENDES, Applied Physics, NOE ALVAREZ, Dep. Chemistry, HOWARD SCHMIDT, R. Smalley Inst., MATTEO PASQUALI, Dep. Chemical and Biomolecular Eng., Rice Univ. — We theoretically investigate the separation of individualized metallic and semiconducting SWNTs in a dielectrophoretic (DEP) flow device. The SWNTs motion is simulated by a Brownian Dynamics (BD) algorithm including the translational and rotational effects of hydrodynamic, Brownian, dielectrophoretic, and electrophoretic forces. The device geometry is chosen to be a coaxial cylinder, because it yields effective flow throughput, and all fields can be described analytically. We construct a flow-DEP phase map, showing different regimes depending on the relative magnitudes of the forces in play. The BD code is combined with an optimization algorithm that searches for the conditions which maximize the separation performance. The optimization results show that a 99% performance can be achieved with typical SWNT parameters by operating in a region of the phase map where metallic SWNTs orient with the electric field, whereas the semiconducting SWNTs flow align. We show spectroscopic measurements of experimental tests which demonstrate metallic vs. semiconductor separation at frequencies in the MHz range. These results reveal crucial knowledge on the influence of the surfactant on the SWNTs effective conductivity.

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