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Self-consistent numerical simulation of carbon transport in the arc discharge for carbon nanotube synthesis¹ ALEXANDER KHRABRY, AN-DREI KHODAK, Princeton Plasma Physics Laboratory, Princeton, NJ, KENTARO HARA, Texas AM University, College Station, TX, VALERIAN NEMCHINSKY, Keiser University, Fort Lauderdale, FL, IGOR KAGANOVICH, Princeton Plasma Physics Laboratory, Princeton, NJ — In carbon nanotube synthesis in the arc, graphite anode ablates providing carbon material into the arc core. Most of the carbon material deposits onto a surface of cathode, whereas some part of it escapes from the inter-electrode gap, cools down and serves as a feedstock for growth of nanoparticles. Carbon atoms associate into carbon dimers, trimmers, etc. with the dimers being the main precursor for growth of carbon nanotubes. Ablation rate is very sensitive to such arc parameters as arc current and gap width. Numerical simulations of carbon arc were performed using self-consistent model which couples effects of fluid flow, carbon transport, current flow, and heat transfer in both plasma and electrodes. Plasma model accounts for non-equilibrium conditions in the arc including effects of space-charge sheaths and solves separate transport equations for ion and neutral species. The arc model was implemented into general-purpose CFD-code ANSYS CFX, which was highly customized for this purpose. Very good agreement between simulation results and experimental data [1] on ablation/deposition rates and density profile of carbon dimers were obtained. [1] V. Vekselman et.al., Plasma Sources Sci. Technol. (2017)

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