GEC20-2020-000455

Abstract for an Invited Paper
for the GEC20 Meeting of
the American Physical Society

Integrated Modeling of Carbon and Boron Nitride Nanotubes Synthesis in Plasma of High-Pressure Arc.[1]

IGOR KAGANOVICH, Princeton Plasma Physics Laboratory

In our previous experiments we synthesized boron nitride (BNNTs) and carbon nanotubes (CNTs) in volume by anodic arc discharges at near atmospheric pressure of nitrogen and helium, respectively. In order to understand NT formation, we determined the plasma and gas composition in the nucleation and growth regions using laser diagnostics, atomistic simulations, thermodynamic and fluid dynamics (CFD) modeling. Firstly, we performed validated arc modeling to predict how the arc can provide feedstock for nanomaterial synthesis. A complicated setup was implemented into ANSYS and included many complex effects: radiation, sheath boundary conditions near emitting electrodes, ablation/deposition of carbon on electrodes, and coupling of the thermal transport through electrodes. In addition, we developed several analytic models for key phenomena: 1) nonlinear dependence of the ablation rate as a function of arc current and interelectrode gap, 2) anode spot formation, in which the arc channel is constricted near anode, 3) radial narrow arc jet emanated from the arc. Thermodynamic modeling results show that at a temperature of 3000K, where CNT are thermally stable, carbon condenses into the long chains and then rolls into flakes and further converts into fullerenes. Therefore, the only carbon available for CNT formation is the carbon dissolved into metal catalyst particles. This also strongly supports the root growth mechanism model. For production of boron nitride nanotubes (BNNTs), boron is evaporated in the near-atmospheric-pressure arc in nitrogen atmosphere. We study precursors for the BNNTs' formation that can effectively convert molecular nitrogen (N_2) into boron nitride. Using quantum chemistry methods, we discovered that formation of linear BNBN, and other more complex BN species from small boron clusters and N_2 proceeds through many sequential steps with activation barriers. Thus, based on our calculations we can conclude that N_2 is able to react with small boron clusters producing new BN clusters, and these clusters can be accumulated in the gas phase even at high temperature providing contribution to the BNNTs' growth.

[1]This research was performed at the Princeton Collaborative Research Facility (PCRF) at PPPL and supported by the US DOE under contract DE-AC02-09CH11466.