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Determination of BNNT growth precursors using thermodynamic analysis[1] ALEXANDER KHRABRY, SHURIK YATOM, IGOR KAGANOVICH, VLADISLAV VEKSELMAN, YEVGENY RAITSES, Princeton Plasma Phys Lab — Recent works [1], [2] demonstrated high-yield production of high-quality boron-nitride nanotubes (BNNTs) in ICP plasma and laser ablation reactors. Common vision on the BNNTs growth is a root-grow mechanism. When B-N gas mixture cools down, boron droplets form first. Then, boron within the droplets reacts with nitrogen-containing radicals from the ambient gas, and BNNTs grow at the droplets surfaces. Ab-initio molecular dynamic simulations [3] have witnessed in favor of this mechanism. However, what are the gas species that provide nitrogen for the BNNTs growth, is still and open question. To determine these precursors, we performed thermodynamic calculations of the gas composition. Broad set [4] of molecular species was considered, condensation of boron was taken into account. We show that B_2N molecules are the major nitrogen source. The presence of B_2N molecules in the gas was confirmed in our experiments using optical emission spectroscopy (OES) of a gas over laser-ablated boron-rich targets. With addition of hydrogen, NH and BH molecules serve as nitrogen sources, which accords with OES measurements [1]. [1] K.S. Kim et al., ACS Nano **12** (2018) 884. [2] R. Arenal et al., J. Am. Chem. Soc. **129** (2007) 16. [3] B. Santra et al., arxiv.org/pdf/1803.11374.pdf (2018). [4] J. Radic-Peric, Mater. Sci. Forum **518** (2006) 349.

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