Abstract Submitted
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DFTB+ simulation of B_xN_y species formation for boron nitride nanotubes synthesis[1] OMESH DHAR DWIVEDI, Princeton Plasma Physics Laboratory and Drexel University, YURI BARSUKOV, Saint-Petersburg Polytechnic University, Russia, IGOR KAGANOVICH, SIERRA JUBIN, STEPHANE ETHIER, Princeton Plasma Physics Laboratory, PRINCETON COLLABORATIVE LOW TEMPERATURE PLASMA RESEARCH FACILITY (PCRF), PPPL TEAM — Using DFTB+ MD simulations we analyze B_xN_y species formation in a cooling mixture of boron atoms and nitrogen dimer. These species could be precursors of boron nitride nanotubes (BNNTs) synthesis. We determine that DFTB+ cannot predict correctly reaction of boron atoms and boron dimers with nitrogen molecules. The first reaction produces BN_2 molecule and simulations show it to be stable, even at T ¿ 3000K. This is incorrect since BN_2 molecule dissociates into B and N_2 from the $^2B_2$ state which has higher energy than $BN_2(^2A_1)$. DFTB+ is not able to reproduce transition from $^2A_1$ to $^2B_2$ state. Similarly, stable BNBN molecule is difficult to observe in these simulations, since the reaction leading to formation of BNBN has a high energy barrier and is kinetically hindered. Nevertheless, DFTB+ simulations show formation of planar B_2N_2 and BBN_2 molecules and larger clusters (B_3N_3 , $B_{12}N_{12}$, etc). Finally, we analyze the thermodynamic feasibility of these reactions through minimization of Gibbs Energy of formation.

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