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Challenges for Growth of Smallest Diameter Single-Walled Carbon Nanotubes by Catalytic Method OLEG KUZNETSOV, ELENA MORA, TOSHIO TOKUNE, Honda Research Institute USA Inc., STEFANO CURTAROLO, Duke University, KIM BOLTON, Goteborg University, AVETIK HARUTYUNYAN, Honda Research Institute USA Inc., HONDA RESEARCH INSTITUTE USA INC. TEAM, DUKE UNIVERSITY TEAM, GOTEBOG UNIVERSITY TEAM — We investigate the viability of formation of very small diameter ($< 0.5\text{nm}$) freestanding SWNTs by CVD based on concept of carbon diffusion through the catalyst particle, originated from the vapor-liquid-solid growth mechanism. We found that the decrease of particle size required for nucleation of small diameter tubes results in a significant increase of catalytic decomposition temperature of hydrocarbon and, accordingly, the temperature required for nucleation and growth of nanotubes. However, high temperature increases the mobility of particles and endorses their agglomeration with formation of bigger particles, as well as leads to deactivation of catalyst by formation of intermetallic compounds with support material. The results of Raman spectroscopy, (n,m) assignments of the grown tubes and TEM studies for the smallest diameter tubes are presented. Performed *ab-initio* and molecular dynamics simulations qualitatively explain the experimental finding based on size dependent carbon solubility of catalyst, by analyzing supported nanocatalyst-carbon binary phase diagram.

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