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Modeling and simulation of arc discharges for nanoparticle synthesis[1] MADHUSUDHAN KUNDRAPU, JIAN LI, ALEXEY SHASHURIN, MICHAEL KEIDAR, The George Washington University — Arc discharge can produce nanoparticles with fewer topological defects. In order to improve the controllability of synthesis, a comprehensive understanding of the growth mechanism of nanoparticles is required. Experimental investigation has limitations in measuring the required parameters especially, species density and temperature distribution. Hence, a self-consistent numerical model is developed to simulate arc discharge chamber. Simulations are performed for arc current varying from 10 to 100 A with 4 mm electrode-gap in Helium background at 68 kPa. The sublimation rate and current-voltage characteristics are compared with the experiments. Good agreement is observed between simulation and experiment results. The probable growth region of nanoparticles is identified and Gibbs free energy model is then used to estimate the critical cluster size and further growth of nanoparticles. The catalyst cluster sizes are compared with those obtained from the TEM images of the experiments. Parametric studies are carried to indentify the inputs for which better growth is achieved.

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