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Size control, transport, and collection of nanoparticles grown in pulsed hollow cathode discharge: Theory and modeling

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The progress in theory and modeling is reported for a project based on nanoparticle (NP) synthesis using pulsed hollow cathode (HC) discharges. In this technique NPs nucleate in high density plasma clouds ejected from the HC, and then grow mainly by the collection of ions of the sputtered material. Different approaches are needed in a sequence of five stages: (I) the production and ionization of sputtered material ejected from the HC, (II) the nucleation and early growth of NPs which have no charge, in our case up to about 1 nm radius, (III) the continued growth to the final size of NPs that acquire a negative charge, (IV) the transport of these NPs from the growth zone to the substrate vicinity, and (V) the final attachment to a substrate. Stage (I) is modeled by a global plasma-chemical model combined with COMSOL. The nucleation rate in stage (II) is treated as a free parameter, to be based on experimental data. For the calculation of the NP charge and growth in stage (II), accurate values of the size- and material dependent electron affinity and work function are needed. These are obtained by separate density functional theory modeling and used to quantify thermo-ionic emission (TIE) and electron field emission (EFE). In stage (III) both TIE and EFE are shown to be negligible below a critial NP tempearature, and above a critial NP size. For this case the NP growth is modeled based on orbit motion limited theory, combined with collision-enhanced collection of ions. The transport in stage (IV) is assessed analytically and modeled by COMSOL, which reveals an interplay between Brownian motion, electric fields, and gas flow drag, with a relative importance that depends on the NP size and charge. For the collection phase (V) on substrates, particle agglomeration or aggreagation both need to be considered as they will affect the types of structures formed.

Keywords
nanoparticles
HC discharges
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