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Controlled Growth of Silver Nanoclusters: A Molecular Dynamic Study MINE KONUK, Department of Physics, Istanbul Technical University, Istanbul, Turkey, SONDAN DURUKANOGLU, Faculty of Engineering and Natural Sciences, Nanotechnology Research and Application Center, Sabanci University, Istanbul, Turkey — We have investigated the growth processes of various Ag nanoclusters with different shape and morphology. In order to understand the shape evaluation of nanocluster at the atomistic level, the energy barriers and reaction rates of different pathways are determined using nudged elastic band method and molecular dynamic simulations based on the potentials extracted from embedded atom method. Growth processes are controlled using varying initial nucleation conditions: deposition angle and rate, temperature, cluster size and shape. Our results show that the reaction conditions control the formation of atoms into clusters and determine the shape of nanocrystals. We also discuss our simulation results with the experimental studies based on the shape-controlled synthesis.

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