Simulation of Silica Cluster Overcharging

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The interaction of an e-beam with silica glass has been simulated using the $27SiO_2$ cluster, charged from 0 to −18 by a PM3 semiempirical quantum chemical method. The structures of the charged $27SiO_2$ silica clusters and their physicochemical characteristics, namely the heat of formation, relative volume, electron density of states distribution, gap between HOMO and LUMO and charge distribution, have been derived and analyzed in order to study the processes occurring on the atomic level at an e-beam-irradiated surface. The overcharging of the silica cluster led to its expansion by 30% in volume and evaporation of the charged species, followed by cluster densification. The silica cluster expansion should lead to structural changes in the neighbouring silica glass areas.

Key words: Silica Glass; E-Beam Irradiation; Computer Simulation; EDOS.