

Abstract Submitted
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Effect of hydrogen coating on the shape of silicon nanoclusters¹

TAKUMI HAWA, MICHAEL ZACHARIAH, University of Maryland and National Institute of Standards and Technology — The effect of hydrogen coating on the shape of silicon nanoclusters has been investigated using molecular dynamics simulation. We use Kohen-Tully-Stillinger potential to model the Si-H system. We consider bare and hydrogen coated silicon nanoclusters, which have crystal structure of cubic and truncated octahedron shapes and amorphous spherical shape for sizes between 2 nm and 10 nm. For bare Si clusters, truncated octahedron clusters are the most stable shape and amorphous spherical clusters are the least stable shape. On the other hand, cubic clusters are the most stable shape and amorphous spherical clusters are the least stable shape for hydrogenated Si clusters. Transition of the cluster shape was also observed from the MD simulation. This prediction explains the production of cubic Si clusters in the plasma synthesis.

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