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Modeling the Melting of Free and Supported Metal Clusters[1] KIM BOLTON, Physics Department, Goteborg University, SE-412 96, Goteborg, Sweden; School of Engineering, University College of Boras, SE-501 90, Boras, Sweden, FENG DING, MEMS Department, Rice University, MS 321, Houston, TX 77005, HAIMING DUAN, ARNE ROSEN, Physics Department, Goteborg University, SE-412 96, Goteborg, Sweden, AVETIK R. HARUTYUNYAN, TOSHIO TOKUNE, Honda Research Institute USA Inc., 1381 Kinnear Road, Columbus, OH 43212, STEFANO CURTAROLO, Department of MEMS, Duke University, Durham, NC 27708 — The growth rate and mechanism of one-dimensional structures, such as carbon nanotubes and zinc-oxide nanorods, is expected to be significantly affected by the phase of catalytic metal particle. It is therefore important to understand the structure and dynamics of these particles in their solid and liquid phases, and to know how their melting points depend on cluster size and substrate adhesion. Results from molecular dynamics studies on the structural and dynamic changes during melting of free and supported iron clusters, ranging from 150 to 10 000 atoms, will be presented. We will also present a method to determine effective diameters of supported metal clusters, so that the melting point dependence on cluster size can be predicted in a physically meaningful way by the same analytic model used for free clusters.

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