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The Effect of Hydrogen Passivation Surface on Silicon Nanodroplets Coalescence TAKUMI HAWA, The University of Oklahoma — Understanding a fundamental formation mechanism of nanoparticles growth and controlling primary particle size and extent of agglomeration when grown from the gas–phase are the significant challenges in the use of nanoparticles. In this talk a possibly mathematical model to describe the droplet coalescence is presented. Here the coalescence of hydrogen terminated silicon surface slowing the process has been studied, and results are compared with molecular dynamics simulations. Nanodroplets of the size between 2 and 6 nm at 1500 K were considered. The hydrogen passivation surface completely changes and slows the beginning of the coalescence process. In addition, the presence of hydrogen atoms reduces surface tension of the droplet about 40 to 50%. The model is able to describe both initial induction period and the standard coalescence period. It presents that the effective surface tension decreases with increasing hydrogen coverage, making it harder for droplets to coalesce. http://www.ou.edu/mms/

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