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Nanowires nucleation by impact of metallic nanoparticles SERGIO MEJIA-ROSALES, JOEL ANTUNEZ-GARCIA, EDUARDO PEREZ-TIJERINA, Facultad de Ciencias Fisico-Matematicas, Universidad Autonoma de Nuevo Leon, San Nicolas de los Garza, NL, Mexico 66450, MIGUEL JOSE-YACAMAN, Chemical Engineering Department and Texas Advanced Materials Center, The University of Texas at Austin, Austin, Texas 78712 — We performed molecular dynamics simulations of impacts between gold spherical and icosahedral nanoparticles, at different relative velocities, temperatures and orientations. We found that the coalescence process depends not only on the energy supply available for the reconstruction of the structures, but the coalescence times and final equilibrium structures are strongly determined by the relative orientations of the particles at the moment of the impact. For most of the conditions, the resulting particle show a tendency to take a quasi-icosahedral shape with triangular (111) faces but, when two icosahedra are impacted in a face-to-face orientation at 300m/s and T=350K, the resulting structure is elongated on the impact direction. A quiral elongated structure results from the impact of two spherical particles, and this geometry survives even after the impact of a third particle. The stability of these structures may be of importance for the nucleation of metal nanowires. Finally, we made a comparison of the simulation results with TEM observations.

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