

Atomistic investigation of the oxidation and laser synthesis of nickel nanoparticles

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Nickel nanoparticles (NiNPs) exhibit unique magnetic and chemical properties that make them attractive for applications in catalysis, sensing, and nanotechnology. In this study, reactive molecular dynamics simulations were used to investigate the oxidation behavior of NiNPs in oxygen-rich environments, focusing on the roles of particle size, temperature, and pulsed thermal excitation. The results reveal that oxidation proceeds via a surface-limited mechanism, with reaction rates increasing systematically with nanoparticle diameter and temperature. Simulated pulsed heating, designed to mimic femtosecond laser excitation, significantly enhances oxidation by inducing transient high-temperature conditions that promote irreversible surface reactions. These findings provide fundamental insight into the size- and temperature-dependent oxidation dynamics of NiNPs and underscore the importance of laser-induced thermal histories in controlling their reactivity during laser-based processing or synthesis.

Keywords : Nanoparticles, Laser, Oxidation, Molecular Dynamics.

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