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Molecular Dynamics Simulations of Super Heated Ni_4 Cluster

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Abstract: The fragmentation mechanism of the super heated Ni4 cluster is studied by employing the microcanonical molecular dynamics simulations and an empirical model potential. Ni_4 cluster is heated up above the bulk Ni evaporation point temperature and then classical trajectory analysis as well as RRK theory are used to calculate survival probability, evaporation rate, average kinetic energy release and dissociation energy.

Key Words: microcanonical molecular dynamics, cluster fragmentation.

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