Temperature evolution of structural and magnetic properties of large Ni clusters

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Tight Binding Molecular Dynamics (TBMD) simulations and additional ones using a variety of classical potentials, incorporating the Nosé-Hoover equations, h ave been used for studying the temperature evolution of structural and magnetic properties of small Ni clusters and the results of this study are presented. Using these results for the small Ni clusters, we present a new method which combines tha classical potentials (which reproduce the TBMD results for the small clusters), with the Tight Binding Hamiltonian and makes possible a calculation of quantum mechanical quantities, such as the temperature evolution of the magneti moment of large clusters. This calculation is imposible with the pure TBMD due to the extremly large time needed for the calculations. Within this treatment, we present our results for the temperature evolution of the magnetic moment of large Ni clusters and some other thermodynamic quantities such as caloric curve, melting temperature, specific heat etc.