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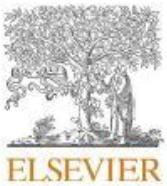

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Research article

A theoretical model to predict the Curie and Neel temperatures of Ni and Fe_3O_4 nanostructured magnetic materials

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ABSTRACT

A simple and unified model, based on size, shape, and surface effect is reported to estimate the magnetic properties of Ni and Fe_3O_4 nanomaterials. The relaxation factor, which is the ratio of dangling bonds to an atom's total bonds, is reported in the theory to estimate the properties of magnetic nanomaterials. The Curie temperature is projected to decrease with the decrement in particle size. The particle shape influences the Curie temperature of Ni and Fe_3O_4 nanoparticles and this effect becomes prominent with the reduction in particle size. The model is extended on the same ground to analyze the Neel temperature of Ni and Fe_3O_4 nanomaterials. Neel temperature also decreases as particle size decreases. The variation of Curie temperature and Neel temperature is projected for spherical, cubic, wire, and film shaped nanoparticles. It is also observed that the effect of size is more appreciable when the shape changes from cubic to the film of nanoparticles. Although, model predictions are valid throughout the size range of nanoparticles, but more noticeable up to the size of 20 nm. Moreover, the reported model is valid for all conducting and semiconducting crystalline nanostructured materials. Our theoretical calculations are in agreement with the standing experimental data and the simulation results for nanoparticles in varying shapes and sizes.