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The effect of shape, spin, and grain boundary on the vibrational properties of iron nanoparticles GIRIDHAR NANDIPATI, SAMPYO HONG, TALAT RAHMAN, University of Central Florida — We have performed both spin-polarized and nonspin-polarized density functional theory (DFT) calculations of vibrational modes for Fe113 of either rectangular or spherical shape. We also have calculated them for a spherical nanoparticle with a single grain boundary ($\sum 3(111)$) to understand the effect of grain boundary. We used both classical molecular dynamics and DFT to optimize the geometry of the Fe113 nanoparticles. Regarding the vibrational density of states (VDOS) of the nonspin-polarized Fe nanoparticles, the spherical shape exhibits a slightly enhanced VDOS in high frequency modes as compared to rectangular shape. The grain boundary brings about remarkable changes in the VDOS in all frequency ranges (as compared to the VDOS of Fe nanoparticles without a grain boundary: (1) enhanced VDOS in low frequency range (10-15 meV) (2) peak shift to higher frequency in middle range (20 – 35 meV) (3) new peaks in high frequency range (40 - 55 meV). Most remarkable changes occur when spin is taken into account for Fe113 nanoparticle. The average magnetic moment (per atom) of the spherical Fe113 nanoparticle calculated by DFT is 2.7 Bohr magneton, which is already close to that of iron bulk (2.2 Bohr magneton). The spin-induced features in VDOS (as compared to non-spin cases) are: remarkable (1) increase in the low and middle frequency regions (7-30 meV) and (2) decrease in the high frequency regions. These spin effects are possibly correlated to spin-induced Fe-Fe bond softening (Fe-Fe bond length expansion). Work supported by DOE Grant No. DE-FG02-07ER46354.

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