Structures and magnetic properties of Fe_n (n=1-4) nanowires

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The crystal structures of Fe nanowire synthesized by electrodeposition and encapsulation methods in carbon nanotubes have been identified as single crystal bcc and fcc structures or bcc+fcc polycrystalline structure. There are several recent theoretical studies on the crystal structure of Fe nanowire. Structures and magnetic properties of free-standing Fe_1 and Fe_2 wires were calculated by Fagan *et al.* [1]. Sen *et al.* considered various periodic pentagonal Fe-wires and they obtained the results that the magnetic staggered pentagonal Fe_{12} wire with central chain is energetically more favorable relative to eclipsed and deformed staggered pentagonal wire [2].

The staggered structures are created by rotating a planar geometry along z-axis. We thus expect these geometries to be good candidates for thin free standing Fe-wires. We have investigated thin planar and zigzag Fe_n (n=1-4) wires, in which n indicates the number of atoms in unit cell. The axis of the wire is taken along the z-axis and the lattice parameters of unit cell in the xy-plane are set as 20 Å. We have carried out spin-polarized density functional calculations using ultrasoft pseudopotential plane wave code. All the calculations were performed with GGA of Perdew-Wang 1991, cutoff energy of 297 eV, and 1×1×20 Monkhorst-Pack k-points for Brillouin zone integration. In order to obtain stable Fe-wires, we performed fully relaxing calculations. The geometry was optimized until the atomic forces were smaller than 0.01 eV/Å using conjugate gradient method. From the calculated results, we discuss the relations between the structures and the magnetic properties.

The linear wire has an equilibrium distance of 2.25 Å and magnetic moment of 3.31 μ_B/atom. Same as a previous study [3], the linear Fe_1 wire is a strong ferromagnet in which the majority d-bands is nearly filled below Fermi energy. Total energy minimum point for zigzag Fe_2 wire locates at wire length of 2.50 Å. When the zigzag wire is elongated, a linear chain is formed at wire length of 5.30 Å. The variation of magnetic moment per atom increases with bond length in the region of wire length greater than that of stable geometry. The energy of equilateral triangle Fe_3 wire is 0.77 eV lower than the linear structure. Fe_4 wire composed of staggered dimers is more stable than square wire. Square Fe_4 wire shows a nearly paramagnetic ordering, while zigzag Fe_4 wire is a strong ferromagnet with a magnetic moment of 2.71 μ_B/atom.

References

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