New monoclinic ground state of FeSi

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Abstract: By means of *ab initio* techniques with the hybrid functional we show the existence of a new phase of FeSi with the monoclinic symmetry (space group $P2_1$) originated from the B20 cubic structure (space group $P2_13$) due to slight orthorhombic distortion, which is turned out to be the ground state. The monoclinic FeSi not only displays the minimum in the total energy, but it is also characterized by a phonon spectrum without imaginary frequencies and by conducting properties (contrary to semiconducting properties of cubic FeSi) with antiferromagnetic ordering and the magnetic moment of 2.3 μB for each Fe atom. These findings are supported by data of X-ray diffraction and high-resolution transmission electron microscopy of ultrathin FeSi films (~3nm in thickness) grown on Si(111) by solid-phase epitaxy indicating the monoclinic symmetry to fit better the film structure as compared to the cubic symmetry, as well as by resistivity versus temperature measurements within a wide temperature range (2–300 K) pointing out bad metal properties. The analysis of field and temperature dependences of the magnetic moment of ultrathin FeSi films shows the presence of a ferromagnetic-antiferromagnetic two-phase state. We also discuss how our findings of the new phase of FeSi can interpret its known experimental data on electronic, transport and optical properties without involving the metal–insulator transition and Kondo-like effects.

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