Abstract First-principles calculations, based on density functional theory (DFT), are used to study the phase stability, elastic, magnetic, and electronic properties of cubic (c) Fe_4C. Our results show that c-Fe_4C has ferromagnetic (FM) ground state as compared with antiferromagnetic (AFM) and nonmagnetic (NM) states. To study the phase stability of c-Fe_4C, BCC Fe_4C, FCC Fe_4C, and BCC $Fe_{16}C$, where C is considered at tetrahedral and octahedral interstitial sites, are also considered. The formation energy of c-Fe_4C is smaller than BCC Fe_4C but the shear moduli ofc-Fe_4C is negative in both the FM and AFM states indicating that c-Fe_4C is dynamically not stable in the magnetic (FM/AFM) state. NM state has positive shear moduli which illustrates that the instability in c-Fe_4C is due to magnetism and can lead to soft phonon modes. The calculated formation energy also shows that c-Fe_4C has higher formation energy than the FCC Fe_4C indicating no possibility of c-Fe_4C in low carbon steels at low temperature. The magnetic moment of Fe in c-Fe_4C is also sensitive to lattice deformation and the electronic structure reveals the itinerant nature of electrons responsible for metallic behavior of c-Fe_4C.

Keywords
Elastic properties· Magnetism · First-principles · Ferrous Carbides