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INVITATION

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Silicon-based layers: experimental study and applications

by

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First-principles calculations, based on density functional theory (DFT), are used to study the phase stability, elastic, magnetic, and electronic properties of cubic (c) Fe4C. Our results show that c-Fe4C has ferromagnetic (FM) ground state as compared with antiferromagnetic (AFM) and nonmagnetic (NM) states. To study the phase stability of c-Fe4C, BCC Fe4C, FCC Fe4C, and BCC Fe16C, where C is considered at tetrahedral and octahedral interstitial sites, are also considered. The formation energy of c-Fe4C is smaller than BCC Fe4C but the shear moduli ofc-Fe4C is negative in both the FM and AF states indicating that c-Fe4C is dynamically not stable in the magnetic (FM/AFM) state. NM state has positive shear moduli which illustrates that the instability in c-Fe4C is due to magnetism and can lead to soft phonon modes. The calculated formation energy also shows that c-Fe4C has higher formation energy than the FCC Fe4C indicating no possibility of c-Fe4C in low carbon steels at low temperature. The magnetic moment of Fe in c-Fe4C is also sensitive to lattice deformation and the electronic structure reveals the itinerant nature of electrons responsible for metallic behavior of c- Fe4C.

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