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Physical properties investigation of $Fe_{1?x}Al_x$ (x?50%-at) alloys using DFT and Wagner-Schottky model

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Abstract: Atomistic modeling based on the Density Functional Theory (DFT) is used to study thestructural, magnetic, electronic and mechanical properties of $Fe_{1?x}Al_x$ alloys (x?50%-at) with and without B, C and N additions over the selected range of Al atomic concentration. It is shownthat a singularity around x Al ? 40%-at is observed for the lattice parameters while the magneticmoment decreases uniformly without unexpected trend. The enthalpies of formation indicatethat the presence of B stabilizes the system for Al concentration in the range of 25%-at<xAl<45%-at and the electronic properties are affected by B, C and N additions. The trends inYoung modulus, bulk modulus, expected ductility (Pugh ratio) and Vickers hardness evolutionare also estimated. N addition improves the Young modulus of alloy while C addition increasesits ductility. By using the Wagner-Schottky model, temperature and composition dependences ofthermal vacancies in B2-FeAl reveal that the double defect Al Fe anti-sites and Fe vacancies aredominating in the Al-rich side at finite temperature. In addition, the diffusion phenomenon isobserved for B, C and N atomic defects.

Keywords : iron aluminides, Magnetic Properties, elastics proprieties, Electronic structures, DFT calculations, thermal defects, Wagner-Schottky Model