

# Physical properties investigation of $\text{Fe}_{1-x}\text{Al}_x$ ( $x \leq 50\%$ -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 the structural, magnetic, electronic and mechanical properties of  $\text{Fe}_{1-x}\text{Al}_x$  alloys ( $x \leq 50\%$ -at) with and without B, C and N additions over the selected range of Al atomic concentration. It is shown that a singularity around  $x \text{ Al} \approx 40\%$ -at is observed for the lattice parameters while the magnetic moment decreases uniformly without unexpected trend. The enthalpies of formation indicate that the presence of B stabilizes the system for Al concentration in the range of  $25\% \text{-at} < x \text{ Al} < 45\% \text{-at}$  and the electronic properties are affected by B, C and N additions. The trends in Young modulus, bulk modulus, expected ductility (Pugh ratio) and Vickers hardness evolution are also estimated. N addition improves the Young modulus of alloy while C addition increases its ductility. By using the Wagner-Schottky model, temperature and composition dependences of thermal vacancies in B<sub>2</sub>-FeAl reveal that the double defect Al-Fe anti-sites and Fe vacancies are dominating in the Al-rich side at finite temperature. In addition, the diffusion phenomenon is observed for B, C and N atomic defects.

**Keywords :** iron aluminides, Magnetic Properties, elastic properties, Electronic structures, DFT calculations, thermal defects, Wagner-Schottky Model