

Nitriding effect on structural stability and magnetic properties of FeAl alloys: DFT study

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Abstract: Using the DFT calculations, the phase stability, structural deformation and magnetic moment of Fe-rich FeAl alloys in presence of different percents of nitrogen were calculated. The formation enthalpy of these Fe-Al alloys indicates that N preferred the octahedral site than the substitution one. Significant changes occur in this energy, affected by N and Fe content causing local distortions. From 25 at.% N, the phenomenon of saturation appeared and the substitution takes place. The addition of 6 at.% N stabilizes Fe₉Al₇ and Fe₁₀Al₆. The presence of N atom leading to decrease the total magnetic moment of FeAl nitride when the magnetic order is antiferromagnetic between N and Fe atom. This magnetic moment increased by the ferromagnetic coupling between Fe and N, thus increasing the Fe local magnetic moment and the magneto-volume effect.

Keywords : Nitriding, Magnetic Properties, Structural Stability., FeAl Alloys, DFT