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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 momentof Fe-riche FeAl alloys in presence of different percents of nitrogen were calculated. Theformation enthalpy of these Fe-Al alloys indicates that N preferred the octahedral site than thesubstitution one. Significant changes occur in this energy, affected by N and Fe contentcausing local distortions. From 25 at.% N, the phenomenon of saturation appeared and thesubstitution takes place. The addition of 6 at.% N stabilizes Fe 9 Al 7 and Fe 10 Al 6 . The presenceof N atom leading to decrease the total magnetic moment of FeAl nitride when the magneticorder is antiferromagnetic between N and Fe atom. This magnetic moment increased by theferromagnetic coupling between Fe and N, thus increasing the Fe local magnetic moment andthe magneto-volume effect.

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