



Ab initio lattice stability and elastic properties of Fe-Mn based alloys

By Thomas Gebhardt

Shaker Verlag Feb 2012, 2012. Taschenbuch. Book Condition: Neu. 210x148x mm. Neuware - Fe-Mn based alloys exhibit fascinating properties for a wide range of applications. Fe-Mn alloys can be seen as prototypes for high-Mn steels, featuring high strength and exceptional plasticity due to various metal-physical deformation mechanisms under mechanical load, providing therefore great potential for structural components in automotive engineering. The stacking fault energy (SFE) of the face-centered-cubic (fcc) phase, strongly affected by the chemical composition, governs the deformation behavior and hence the mechanical properties. In a first part of this thesis, the influence of the magnetic state on the lattice stability of fcc vs. hcp Fe-Mn random alloys with and without additions of Al and Si was studied using ab initio calculations. The ab initio results are consistent with thermodynamic calculations, obtained with Calphad. With room temperature magnetic configurations, the cross-over between E_{hcp} and E_{fcc} of binary Fe-Mn alloys is in the expected Mn range and the increase of SFE below the Néel temperature due to additions of Mn is well displayed. The addition of Al strongly stabilizes the fcc lattice below the fcc Néel temperature, which is consistent with an increase in SFE, whereas adding Si yields a...



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