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STACKING FAULT ENERGIES IN AUSTENTIC STEELS FROM DENSITY FUNCTIONAL THEORY

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FeMn-based austenitic steels have attracted great interest due to their superior ductility and strength under mechanical stress. Their deformation behavior has been related to the magnitude of the stacking fault energy (SFE) which is defined as the energy difference between the ideal fcc structure and the intrinsic stacking-fault structure. The former has ...ABCABCABCA... stacking along the [111] direction, while the latter exhibits a single planar defect that changes the fcc stacking into ...ABCAB|ABCA..., due to the slip of Shockley partial dislocations along the [112] direction. When the SFE is smaller than 20 mJ/m2, a process called transformation induced plasticity (TRIP) is observed, whereas for larger SFEs, twins are formed in twinning induced plasticity (TWIP). Measurements of the SFE are, however, cumbersome and scarce, which has motivated its calculation using thermodynamic approaches as well as ab-initio electronic structure calculations.

In this presentation, it will be outlined how the SFE can be calculated from density functional theory. First, it is shown how interstitial carbon atoms influence the SFE by employing a super cell approach within an all-electron full-potential framework. Second, the influence of Mn-concentration and temperature on the SFE in FeMn alloys is discussed. To this end, chemical and magnetic disorder are treated within the coherent potential approximation (CPA) and the disordered local moment (DLM) theory, respectively. The importance of temperature dependent magnetic moments and their contribution to the entropy is emphasized leading to composition and temperature dependent SFEs in good agreement with available experimental data.