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Magnetic Landau free energy density for the bcc-hcp phase transformation MAHDI SANATI, Texas Tech Univ, ROBERT C. ALBERS, TURAB LOOKMAN, AVADH SAXENA, Los Alamos National Lab. — We have studied the bcc-hcp phase transformation in Fe and Co with the use of first-principles calculations. The complete energy surface as the system goes from the bcc to hcp structure is determined. The results are used to find an appropriate Landau free energy (LFE) density for describing this transformation. The Landau free energy consists of three order parameters: shear, shuffle, and magnetization. The coefficients of the Landau free energy density are obtained from first-principles energy fits. The stability of the bcc phase in both elements has been studied and the results are then extended to understand the stability of the bcc Fe-Co alloys with varying stoichiometry.

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