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Competition between magnetic structures in the Fe-rich fcc FeNi alloys IGOR ABRIKOSOV, ANDREAS KISSAVOS, FRANCOIS LIOT, BJORN ALLING, SERGEI SIMAK, Department of Physics, Chemistry and Biology, Linkoping University, Sweden, OLEG PEIL, ANDREI RUBAN, Applied Materials Physics, Royal Institute of Technology, Sweden — We report on the results of a systematic *ab initio* study of the magnetic structure of Fe rich fcc FeNi binary alloys for Ni concentrations up to 50 at. %. Calculations are carried out within density functional theory using two complementary techniques, one based on the Exact Muffin-Tin Orbital theory within the coherent potential approximation and another one based on the Projector Augmented-Wave method. We observe that the evolution of the magnetic structure of the alloy with increasing Ni concentration is determined by a competition between a large number of magnetic states, collinear as well as non-collinear, all close in energy. We emphasize a series of transitions between these magnetic structures, in particular we have investigated a competition between disordered local moment configurations, spin spiral states, the double layer antiferromagnetic state, and the ferromagnetic phase, as well as the ferrimagnetic phase with a single spin flipped with respect to all others. We show that the latter should be particularly important for the understanding of the magnetic structure of the Invar alloys.

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