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Effects of local atomic environment and atomic long range order on magnetism in Fe-Al alloys SERGII KHMELEVSKYI, CMS, Institute for Applied Physics, Vienna University of Technology — Using first-principle Local Self-Consistent Green Function (LSGF) method and Local Spin Density Approximation we have studied local environment effects on magnetism of Fe in FeAl alloys near and at 1:1 atomic composition. The long range atomic order (LRO) in the alloys has been varied from complete disorder (A1) to full order (B2). We have derived the dependence of the Fe magnetic moments on local atomic environment up to second nearest neighbor (NN) shell, which is found to exhibit a highly not-trivial behavior. In order to explain a sharp difference in the magnetic behavior of ordered and disordered Fe-Al alloys we calculate the inter-atomic magnetic exchange interactions and their dependence on the state of the atomic LRO using conventional Lichtenstein formalism. We have found strong antiferromagnetic interactions between Fe atoms on long distance NN shells of underlying bcc lattice, which compete in size with ferromagnetic one on the first NN shells. The magnitude of these interactions is strongly depending on the state of the atomic LRO and this effect is the reason for onset of few different spin-glass regimes in the partially ordered Fe-AL alloys.

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