Influence of the temperature-dependent electron-energy spectrum realignment on the formation of homogeneous magnetic short-range-ordered regions in disordered b.c.c. alloys

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Formation of the homogeneous magnetic short-range-ordered regions in disordered b.c.c. alloys under the influence of the electron-energy spectrum realignment with a temperature is considered. For the description of electron states in a crystal, the multiband model of a tight binding and the developed method for the cluster expansion for Green's functions and thermodynamical potential of a disordered crystal are used. Within the scope of the mentioned approach, the calculations of both the electron-energy spectrum and the temperature dependence of equilibrium values of the pair-wise magnetic-correlation parameters of disordered b.c.c.-$Fe_{0.5}Co_{0.5}$ alloy are performed. The equilibrium values of parameters of magnetic and interatomic correlations are obtained from the condition that a free energy is minimal. Strong correlations between electrons in conditions of their strong Coulomb repulsion and the well-developed short-range order of substitutional atoms lead to appearance of a quasi-gap in the electron-energy spectrum. The microscopic mechanism of magnetic ordering in a b.c.c. alloy is concerned with both the Fermi-level position within the quasi-gap region and the realignment of the electron-energy spectrum with a change of temperature. The parameters of pair-wise magnetic correlations decrease with the temperature increase that leads to increasing electron density of states at the Fermi level. The equilibrium parameters' values of the pair-wise magnetic correlations at some temperature allow to calculate the respective linear sizes of homogeneous magnetic short-range-order regions in b.c.c. alloys. The result of computation for b.c.c.-$Fe_{0.5}Co_{0.5}$ alloy—namely, a steadily decreasing temperature dependence of the linear sizes of homogeneous magnetic-order regions—conforms to the experimental data obtained by Yu.I. Ustinovshchikov et al.(2003).