CALCULATION OF SOLUTION ENTHALPY OF CARBON IMPURITY IN FE – MN PARAMAGNETIC ALLOYS

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In the framework of electronic density functional theory, we calculated a solution enthalpy of carbon impurity into paramagnetic fcc $Fe-Mn$ alloy. Properties of $Fe-Mn-C$ alloys were described with using the model that takes into account the contribution of thermal magnetic fluctuations in paramagnetic matrix with point defects. This model is generalized for the cases of magnetic and chemical disorder. It was found that in alloys containing Mn, the solution enthalpy of carbon decreases compared to pure gamma-Fe. Also, we analyze various possible factors that can increase the carbon solubility in $Fe-Mn$ alloys.