Abstract Submitted
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Structural γ-ε phase transition in Fe-Mn alloys: a CPA+DMFT study[1] ALEXANDER BELOZEROV, SERGEY SKORNYAKOV, ALEXANDER POTERYAEV, VLADIMIR ANISIMOV, Institute of Metal Physics, 620137 Yekaterinburg, Russia — We study the γ-ε structural transition in paramagnetic Fe-Mn alloys for Mn content from 10 to 20 at.% using CPA+DMFT method. This method employs the coherent potential approximation (CPA) combined with the dynamical mean-field theory (DMFT). The material-specific Hamiltonians in the Wannier function basis are obtained by density functional theory. The electronic correlations are found to play a crucial role in this transition. The calculated transition temperature decreases with increasing Mn content and is in a good agreement with experiment. We demonstrate that in contrast to the α-γ transition in pure iron, the γ-ε transition in Fe-Mn alloys is driven by a combination of kinetic and Coulomb energies. The latter is found to be responsible for the decrease of the γ-ε transition temperature with Mn content.

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