# *Ab-initio* calculations of ordering degree in $Fe_3Si$ alloy doped with Mn and Cr

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$Fe_3Si$ crystallises in the $DO_3$-type structure. Mössbauer spectroscopy indicates that small disorder between B and D sites is present in real materials [1, 2]. It means that some silicon atoms occupy B sites. This disordering is still present, while doping $Fe_3Si$ with chromium [3]. In compound $Fe_{3-x}Mn_xSi$ Mössbauer measurements indicated additionally partial disorder between (A,C) and D sites [4]. So far, we have carried out thorough theoretical investigations concerning $Fe_{3-x}Cr_xSi$ [5-7] and $Fe_{3-x}Mn_xSi$ [8] alloys under assumption that silicon atoms occupy D sites only. Because of some discrepancies between theoretical and experimental results, we suspected that experimentally found disorder should be taken into account. Thus we introduce now in calculations a small disorder between both B-D and (A,C)-D positions. Positions' exchange between only Fe and Si is taken into account. Doping atoms (Cr and Mn) are allowed to occupy only B and (A,C) sites. Ab-initio studies are carried out for pure $Fe_3Si$ and for concentration x=0.125. TB-LMTO-ASA method within LSD approximation is applied.

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[1] J.T.T. Kumaran, C. Bansal, Solid State Commun. **69** (1989) 779
[2] L. Dobrzyński, J. Phys.: Cond. Matter **7** (1995) 1373
[3] K. Szymański, L. Dobrzyński, D. Satuła, Proceedings of the International Conference of Physics, Leuven, Hyperfine Interactions (C) **1** (1995) 76
[4] G.A. Al-Nawashi, S.H. Mahmood, A.F.D. Lehloch, A.S. Saleh, Physica B **321** (2002) 167
[5] M. Pugaczowa-Michalska, A. Go, L. Dobrzyński, S. Lipiński, J. Magn. Magn. Mat. **256** (2003) 46
[6] A. Go, M. Pugaczowa-Michalska, L. Dobrzyński, J. Magn. Magn. Mat. **272-276** (2004) e217
[7] A. Go, M. Pugaczowa-Michalska, L. Dobrzyński, Molecular Physics Reports **38** (2003) 86
[8] A. Go, M. Pugaczowa-Michalska, L. Dobrzyński, will be published.

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