VOLUME EFFECT ON THE MAGNETISM OF $Fe_{3-x}Cr_xAl$

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Fe_{3-x}Cr_xAl alloys, in the range $0 \le x \le 0.5$, crystallise in the DO₃ type structure. The decrease of the magnetic moment of iron with the increase of the chromium concentration was obtained by Mössbauer measurements [1]. However, detailed theoretical investigations [2] for the experimental values of the lattice constant [1] show a little bit different gradient of the total magnetic moment versus lattice constant. Furthermore there is quite unexpected behaviour of magnetic moment of iron atoms on one of the unequivalent positions for which the magnetic moment increases with the concentration of chromium. It is well known that magnetic moment of pure iron depends strongly on the Wigner-Seitz radii [3]. The purpose of this work is to investigate the dependence of the total and local magnetic moments on the lattice constant using the self-consistent spin-polarised TB LMTO method with changing values of the lattice constant in the range of $\pm 15\%$ in relation to the experimental values [2].

- [1] D. Satuła, et al., J. Magn. Magn. Mater. 169 (1997) 240.
- [2] A. Go, et al., Molecular Physics Reports 38 (2003) 86.
- [3] D. Bagayoko, J. Callaway, Phys. Rev. B 28 (1983) 5419.

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 $9.7~\mathrm{cm}$