Interplay of crystal structure preference and magnetic ordering in Cr-Co-Fe-Ni-Al high entropy alloys

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Recently, Korringa-Kohn-Rostoker method with coherent potential approximation (KKR-CPA) was successfully applied to investigate theoretically the crystal structure transition (bcc/fcc) in $CrCoFeNiAl_x$ [1] as well as the superconducting properties in Ta-Nb-Hf-Zr-Ti [2]. In this work, some relations between crystal structure and magnetic ordering in $CrCoFeNiAl_x$ HEAs are discussed in view of the KKR-CPA calculations. Remarkably, it is noticed that the transition between bcc and fcc phases in all analysed alloys is closely related to re-arrangement of the local magnetic moments, namely the magnetic moment on Cr is either parallel (ferromagnetic) or antiparallel (ferrimagnetic) to the magnetic moments of other atoms (Co, Fe and Ni). Finally, the results of KKR-CPA calculations of $CrCoFeNiAl_x$ in 'paramagnetic-like' state are also discussed.

References:

- [1] K. Jasiewicz, J. Cieslak, S. Kaprzyk, J. Tobola, J. Alloys Compd 648, 307 (2015)
- [2] K. Jasiewicz, B. Wiendlocha, P. Korbeń, S. Kaprzyk and J. Tobola , Phys. Stat. Sol. (RRL) 10 (2016)