Poster session:

The effect of magnetism to the elastic constants in the high entropy alloy CoCrFeMnNi

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The high entropy alloy which include all five magnetic 3d-transition metal elements CoCrFeMnNi (Cantor alloy), has a very complex ordered magnetic state at low temperatures. At elevated temperatures the Cantor alloy is in a paramagnetic state and the magnetic excitations and thermally disordered local moments are expected to play an important role.

Here we investigate the influence of the magnetic order and longitudinal spin fluctuations at elevated temperatures on the elastic moduli of this alloy on the first-principle basis.

We employ the Korringa-Kohn-Rostoker (KKR) method along with the coherent potential approximation (CPA), which is an ideally suited methodology to deal with alloys, in the framework of the local spin density approximation (LSDA) and disordered local moment (DLM) approach. We also combine this study with large super-cell calculations and ab-initio studies of the magnetic exchange interactions between different alloy components using the magnetic force theorem.

To learn more about the magnetic ordering in the fcc random alloy $Co_{20}Cr_{20}Fe_{20}Ni_{20}Mn_{20}$, we set up four different magnetic structures within the $L1_0$ crystal structure. The $L1_0$ crystal structure has two basis vectors with the Wyckoff position $1a$ and $1d$, we put only Fe and Mn moments within the CPA spheres for the alloy according to the structures M_1 to M_4 in Fig. 1, where the black arrows correspond to Fe and the blue arrows to Mn contributions.

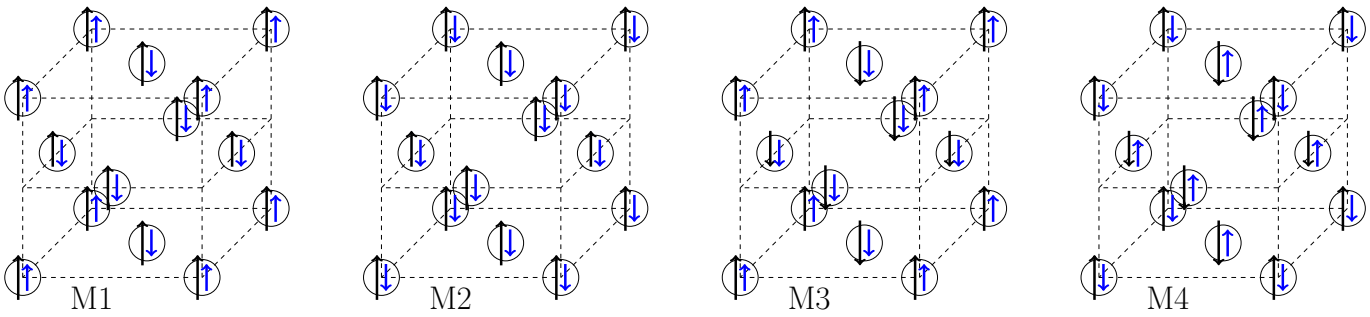

Fig. 1: The four magnetical lattices within the $L1_0$ crystal structure.

Within this magnetic structures M_1 to M_4 we have run fixed spin moment (FSM) calculations. From the total energies of M_1 to M_4 together with the ferrimagnetic and DLM results we learn which one is preferred energetically. We learn that the magnetic structure M_3 has the lowest energy, M_3 corresponds to Fe↑Mn↑ at the $1a$ position and Fe↓Mn↓ at the $1d$ position.

Additionally, we have investigated the influence of the magnetic order and longitudinal spin fluctuations at elevated temperatures on the elastic moduli of the Cantor alloy $Co_{20}Cr_{20}Fe_{20}Ni_{20}Mn_{20}$. We show, in particular, that the dominating magnetic interaction in the system is Fe-Fe and Fe-Mn exchange, which in the absence of the chemical disorder, would lead to the special antiferromagnetic order on the underlying fcc lattice.