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Abstract:

A quenched-in state of thermal equilibrium (at 723 K) in a single crystal of Cr-Fe-Co-Ni close to equal atomic percent was studied. Atom probe tomography revealed a single-phase state with no signs of long-range order. The presence of short-range order (SRO) was established by diffuse x-ray scattering exploiting the variation in scattering contrast close to the absorption edges of the constituents: At the incoming photon energies of 5969 eV, 7092 eV, and 8313 eV, SRO maxima that result from the linear superposition of the six partial SRO scattering patterns, were always found at X position. Electronic structure calculations showed that this type of maximum stems from the strong Cr-Ni and Cr-Co pair correlations, that are furthermore connected with the largest scattering contrast at 5969 eV. The calculated effective pair interaction parameters revealed an order-disorder transition at approximately 500 K to a $L1_2$-type $(Fe,Co,Ni)_3Cr$ structure. The calculated magnetic exchange interactions were dominantly of the antiferromagnetic type between Cr and any other alloy component and ferromagnetic between Fe, Co, and Ni. They yielded a Curie temperature (T_C) of 120 K, close to experimental findings. Despite the low value of T_C, the global magnetic state strongly affects chemical and elastic interactions in this system. In particular, it significantly increases the ordering tendency in the ferromagnetic state compared to the paramagnetic one.

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“Local order in Cr-Fe-Co-Ni: Experiment and electronic structure calculations”

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