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Theoretical Modeling of High Entropy Alloys

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High entropy alloys (HEA) containing Co, Ni, Fe have recently enjoyed considerable attention in the material sciences due to their interesting mechanical and magnetic properties that are further enhanced by the additive manufacturing technique often used to process them.
HEAs are theoretically difficult to describe as they often form amorphous structures and the Bloch theorem is not applicable. In this article the method of the effective medium is used and the corresponding many body problem is solved selfconsistently within the coherent potential approximation. The mixing entropy of HEAs and their phase stability are explained using an optimization approach. The complex micro- and multi phase structure are due to many body effects that are discussed from a calculation of the quasiparticle density of states. It turns out that these many body effects are most significant if the components of the alloy are present at about equal proportions. Applications to Kondo insulators and superparamagnetism are investigated where the interaction between magnetic moments is of indirect type and mediated by the free electrons of the conduction band (RKKY interaction). In the strong coupling limit it is shown that the susceptibility has a maximum at the blocking temperature indicating a phase transition from ferromagnetism to superparamagnetism. Using alternatively a lattice gas model to represent the disordered alloy the existence of the second order phase transition is confirmed and the blocking temperature is calculated. It is shown that the results of the two model calculations are in qualitative agreement with one another and must thus be regarded as good and reliable.

Apply to be considered for a student ; award (Yes / No)?

no

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