Calculation of Curie temperature using the mean-field method of disordered local moments

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The Curie temperature is one of the basic parameters of ferromagnetic materials, which determines the point above which the material loses its magnetic order and becomes paramagnetic. It is also a subtle parameter that is very difficult to determine from first principles. The best results are obtained from Monte Carlo calculations with exchange interactions determined from DFT, but these are computationally very expensive even for relatively simple alloys. A more efficient alternative is the mean-field approach [1,2]. For that we use the equation:

$$k_{\mathrm{B}} T_{\mathrm{C}}^{\mathrm{MFT}} = \frac{2}{3} \frac{E_{\mathrm{DLM}} - E_{\mathrm{FM}}}{c}, \tag{1}$$

where E_{DLM} and E_{FM} are total energies of paramagnetic and ferromagnetic states, k_{B} is Boltzmann's constant, and c is the number of *magnetic* atoms per formula. A ferromagnetic (FM) ground state is easy to calculate as an equilibrium configuration of collinear parallel magnetic moments. In order to calculate the paramagnetic configuration, we used the method of disordered local moment (DLM) [3] based on the coherent potential approximation (CPA) [4]. In DLM approach, we use the approximation originally dedicated to modeling of alloys (CPA) to model a *paramagnetic alloy* composed of two types of atoms with opposite spins and the total magnetic moment equal to zero. While mean-field Curie temperatures obtained this way tend to systematically overestimate experimental values by approximately 20%, the approach is significantly faster than Monte Carlo simulations. Furthermore, combining DLM with a regular CPA allows modeling of the dependence of Curie temperature on concentration.

References:

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