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Transitions ordre-désordre dans les alliages : structure électronique et diagrammes de phase

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The subject treated in this communication has already been published in several places so that we just present here a very brief account and relevant references.

Major advances have been achieved during the last decade concerning the first principles studies of the thermodynamics of alloys. First of all efficient electronic structure methods are now available to calculate ground state energies of ordered compounds, with an accuracy, about 10 mryd/atom, such that energy differences between very similar structures such as e.g. the $L1_2$ and DO_{22} structures become feasible.

On the other hand the energy of any atomic configuration can be obtained through a generalized perturbation expansion providing us with an effective Ising model with concentration dependent interactions. We can then use standard methods of statistical physics (Monte Carlo simulations, simple or sophisticated mean field methods such as the CVM) to determine the phase stability at zero temperature as well as the phase diagrams.

This is fully discussed in a recent book [1]. Other review articles are available [2]. Recent first principles phase diagrams calculations can be found in references [3].

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