A magnetic tight-binding model for metallic alloys

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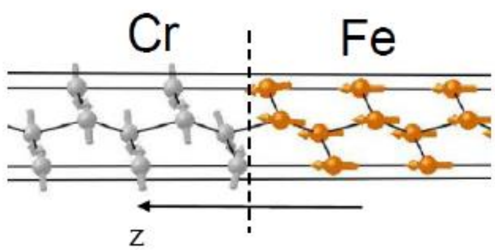

Non collinear magnetic configuration at the (110) interface of FeCr.

In this contribution I will present an efficient tight-binding (TB) model[1] that we have developed to describe the electronic, magnetic and energetic properties of metallic alloys. It is based on a rather simple procedure that only requires a fit on *ab-initio* data of band-structures and energy for single element bulk metals. No specific properties of the binary system is explicitly required. The magnetic part of our TB Hamiltonian is described by a straight-forward spin-dependent Stoner term that can be generalized to deal with non-collinear magnetism and include spin-orbit effects. Usual local charge neutrality condition is applied and simple rules are used to deal with bi-metallic systems.

We have applied this model to a large variety of systems and physical properties. In this contribution I will mainly focus on recent results that we have obtained on FeCr alloys. Our TB model proved to be highly transferable and accurate to describe the complex interplay between magnetism and energetics of FeCr in many structural and chemical environments such as surfaces, interfaces, embedded clusters and over the whole compositional range of the binary alloy. Due to its simplicity and generic approach this model can be applied as well to other magnetic transition metal alloys.

[1] C. Barreteau, D. Spanjaard and M.C. Desjonquères, Comptes Rendus Physique 17, 406 (2016).