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Theoretical study of defected surfaces in CoPt $L1_0$ alloy

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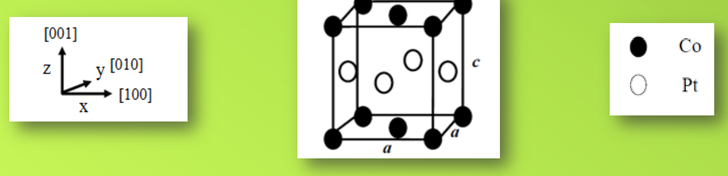
Abstract

The equiatomic CoPt alloy is a promising candidate for ultra high magnetic data recording, due to its tetragonal $L1_0$ structure which has a high uniaxial magnetic anisotropy. In this work we present ab initio study of magnetic properties of defected surfaces in CoPt $L1_0$ alloy, especially surfaces with localized faults, such as antisites. Our results show that the Co (Pt) local magnetic moment does not enhance in the presence of Pt (Co) antisite.

Introduction

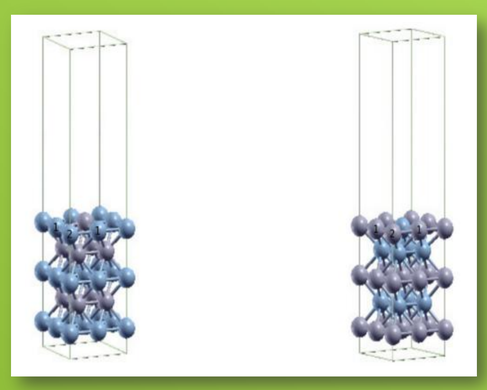
These last years, a prodigious progress has been achieved in the field of ultra-high density magnetic storage device. Under its tetragonal $L1_0$ structure, the CoPt binary alloy may be an ideal candidate for these applications. This structure can be seen as alternating pure Co and Pt planes in the [001] direction [1,2], and has a high magnetocristalline anisotropy [3,4] caused by the combination of exchange and spin-orbit interactions via hybridization of magnetic Co 3d orbitals and Pt 5d orbitals [5]. In this study we had the idea of exploring the case of localized faults, in particular antisites, namely an antisite of Pt in surface of pure Co, and Co antisite within a surface of pure Pt, with a view to highlight new magnetic properties that are likely to appear by changing the environment around a transition metal.



The conventional cell of the CoPt$L1_0$ alloy.

Method

We adopt the slab approach with periodic boundary conditions in two directions while the periodic images in the third direction are isolated by a sufficient amount of vacuum. We have chosen to use non symmetrical calculation cells with odd number of plane, five alternating atomic planes (four atoms per plan) of Co and Pt, as highlighted in figure below. Here, two terminations are possible: either a Co or Pt termination, but the central atom at surface is replaced by the other type of atom; in such a way to have two types of antisites: antisite of Pt in surface of pure Co and antisite of Co in surface of pure Pt.



Supercells used in the surfaces (with antisite) calculations in $L1_0$ CoPt. Left : Slab for the (001), antisite of Pt in surface of pure Co. Right : Slab for the (001), antisite of Co in surface of pure Pt. Blue atoms are Co, magenta atoms are Pt.

Calculation

- Density Functional Theory with Vienna ab initio simulation package (VASP)
- Generalized Gradient Approximation (GGA) with functional from of Perdew, Burke and Ernzerhof (PBE)
- Norm-Conserving Pseudopotentials
- Plane wave energy cut-off fixed to 478 eV
- K-points grids used is 14 x 14 x 1 (Monkhorst Pack)
- A gap region of about 15 Å is used to avoid interaction between neighbouring supercells

Our calculations have been made from a ferromagnetic initial configuration. Here, relaxation and reconstruction concerns only the surface and the subsurface planes, while the others are frozen, respecting bulk distances.

Results of simulation

* We presente in table below the results of magnetic calculation for surfaces with antisite, essentially the contribution of each atom to the total magnetism of supercell.

Plan	Atom	M (μ_B)	Plan	Atom	M (μ_B)
S	Pt antisite	0.32	S	Co antisite	2.01
	Co1	2.04		Pt1	0.42
	Co2	2.02		Pt2	0.39
S-1	Pt	0.40	S-1	Co	1.98
Bulk	Co	1.93	Bulk	Pt	0.41
	Pt	0.39		Co	2.04
	Co	2.04		Pt	0.39

Magnetic profile of surfaces with antisite. Left : Results of magnetic calculation for surface with Pt antisite. Right : Results of magnetic calculation for surface with Co antisite.

* For comparison, we also give the results of our previous study concerning perfect surfaces, and this for two possible case: Co termination and Pt termination

Plan	Atom	M (μ_B)
S	Co	2.04
S-1	Pt	0.40
S-2	Co	1.94
S-3	Pt	0.39
Bulk	Co	1.95
S-3	Pt	0.39
S-2	Co	1.94
S-1	Pt	0.40
S	Co	2.04

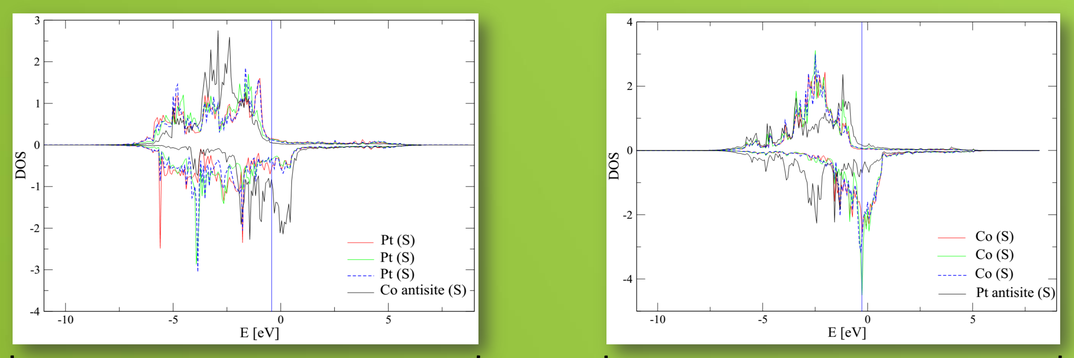
Plan	Atom	M (μ_B)
S	Pt	0.41
S-1	Co	2.03
S-2	Pt	0.40
S-3	Co	1.96
Bulk	Pt	0.39
S-3	Co	1.96
S-2	Pt	0.40
S-1	Co	2.03
S	Pt	0.41

Co termination

Pt termination

* In figure below, we show the atom-projected electronic densities of states (PDOS) for these surfaces with antisite:

We considered only the surface atoms



Pdos of atoms belonging to the surface with Co antisite

Pdos of atoms belonging to the surface with Pt antisite

* These curves of density of states obtained are qualitatively similar to those characteristic of perfect surfaces

Conclusion

In this work, we have investigated the surface properties of the CoPt $L1_0$ binary alloy. We have considered (001) surfaces with localized defects such as antisites, in both Pt antisite in surface of Pure Co and Co antisite in surface of pure Pt.

- Our results on the magnetic properties of Co and Pt atoms are similar to those of perfect surfaces.

- We found that the Pt antisite is extirpated from the surface, unlike the Co antisite which is encrusted in the surface plane.

- We are presently investigating the influence of ad atoms and vacancies, on the physical properties of CoPt $L1_0$ surfaces.

References:
[1] Coffey K R, Parker M A and Howard J K 1995 IEEE Trans. Magn. 31 2737, [2] Alloyeau D, Ricolleau C, Mottet C, Oikawa T, Langlois C, Le Bouar Y, Braidy N and Loiseau A 2009 Nature Mater. 8 940, [3] Weller D and Moser A 1999 IEEE Trans. Magn. 35 4423, [4] Sun S, Murray C B, Weller D, Folks L and Moser A 2000 Science 287 1989, [5] Zemen J, Masek J, Kucera J, Mol J A, Motloch P and Jungwirth T 2014 Journal of Magnetism and Magnetic Materials 356