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Barthélémy Pradines, Rémi Arras, Lionel Calmels. An ab initio study of the effects of vacancies on the static and dynamic magnetic properties of Co₂MnSi. Journal of Physics: Conference Series, 2017, 903, pp.012030. <10.1088/1742-6596/903/1/012030>. <hal-02083169>

HAL Id: hal-02083169

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Submitted on 18 Jun 2019

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To cite this article: B. Pradines *et al* 2017 *J. Phys.: Conf. Ser.* **903** 012030

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An *ab initio* study of the effects of vacancies on the static and dynamic magnetic properties of Co₂MnSi

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Abstract.

The full-Heusler alloy Co₂MnSi is a promising highly spin-polarized magnetic metal for spintronic applications. However, significant differences have been reported between the computed properties of the ideal material and the properties of real samples measured in experiments. In this paper, we study the influence of atom vacancies on the electronic structure and on the magnetic properties of Co₂MnSi, as these defects could explain the disagreement between the expected and measured behavior of this alloy. The effects of atom vacancies have been calculated from first principles, using the fully relativistic Korringa-Kohn-Rostoker (KKR) method in conjunction with the coherent potential approximation (CPA) and the linear response formalism.

1. Introduction

The quest of magnetic materials presenting a half metallic behaviour at high temperatures has intensified during the last 30 years. Defined by the presence of an energy gap in the band structure of only one of the two spin states, this interesting property is sought by the spintronics community, since it would maximize the efficiency of spintronic devices for many applications. With their 100% spin-polarization at the Fermi level, half-metals would for instance provide efficient magnetic electrodes for magnetic tunnel junctions or spin-torque oscillators.

Among all the compounds which have been theoretically predicted as being half-metallic, the full-Heusler alloy Co₂MnSi [1, 2] has managed to get noticed because of its high Curie temperature of 985 K [3] and its Gilbert damping parameter α , lower than 1×10^{-3} [4]. However, the theoretically predicted 100% spin-polarization at E_F of Co₂MnSi has not been yet experimentally confirmed. A value of 93% has been recently measured [5], but most of the previous works announced spin polarization values around 50-60%, at low or room temperature [6, 7, 8, 9]. Furthermore, the values of the Gilbert damping are generally more than 10 times higher than the computed results [10].

Several explanations have been suggested to clarify these qualitative differences between theory and experiment. After confirmation of the presence of atomic disorder in some experimental samples by neutron diffraction experiments [11, 12], chemical disorder became a popular hypothesis to explain the loss of half-metallicity and the high value of α . This hypothesis has further been widely studied in the literature [13, 14, 15]. Another hypothesis advanced by the experimentalist is the presence of vacancies in this material. This latter thesis is well less considered in literature. Özdoğan *et. al* studied numerically the effect of vacancies on each of



the atomic sites of Co_2MnSi [16], and concludes that the half-metallic character of the alloy loses its robustness (large reduction of the minority spin band-gap) when there are vacancies on the Co atomic sites. But numerical studies on the effects of atom vacancies on α are still missing.

For a better understanding of the modification of the physical properties of Co_2MnSi induced by atom vacancies, we have calculated the effect of an increasing density of vacancies, and we only consider here the case of stoichiometric Co_2MnSi alloys, in which vacancies are equitably distributed over all the atomic sites of the alloy. We focus on the effects of vacancies on the electronic structure, the magnetic properties and the Gilbert damping parameter.

2. Calculation details

Our results were obtained using the Korringa-Kohn-Rostoker (KKR) formalism implemented in the spin-polarized relativistic KKR (SPRKKR) code [17]. This program uses the multiple scattering theory to calculate the one-electron Green function of crystals including possible defects via the coherent potential approximation (CPA) [18]. This latter approximation plays a major role in our calculations because it allows to handle the presence of defects like chemical disorder or, in our case, the presence of vacancies with adjustable concentrations on selected atomic sites. Here, we chose to only consider cases where the vacancy concentration is the same for all the atomic sites and where chemical disorder between atomic sites is neglected. A parameter-free expression for α was recently derived by Ebert *et. al.* from the linear response formalism [19]. This technique, contrary to previous methods for calculating α [20, 21], is fully *ab initio* and does not involve any phenomenological parameter accounting for the finite lifetime of the electron states.

The crystal structure of Co_2MnSi is described by the space group $Fm\bar{3}m$ for the perfectly ordered L_{21} phase. In this phase, the Co (X site), Mn (Y site) and Si (Z site) atoms occupy respectively the 8c, 4a and 4b positions of Wyckoff. To account for the effects of vacancies on each atomic site, the following chemical formula was used: $([\text{Co}_{1-x}]_X)_2[\text{Mn}_{1-x}]_Y[\text{Si}_{1-x}]_Z$ where $x \leq 5\%$ is the percentage of vacancies by atomic site. The results presented in the next section were calculated with the local spin-density approximation (LSDA), with the exchange-correlation potential of Vosko, Wilk and Nusair [22] in fully relativistic mode at 0 K. We sampled, after convergence tests, the first Brillouin zone with 3000 k vectors and set up the selected l -cut-off l_{max} of the KKR formalism to 4. A volume optimization was then performed for the perfect L_{21} phase and for the phase with 5% of vacancies per atomic site, the minimum value of the ground state energy was found for $a_0^{\text{DFT}} = 5.48 \text{ \AA}$ in both case and will be used throughout this paper.

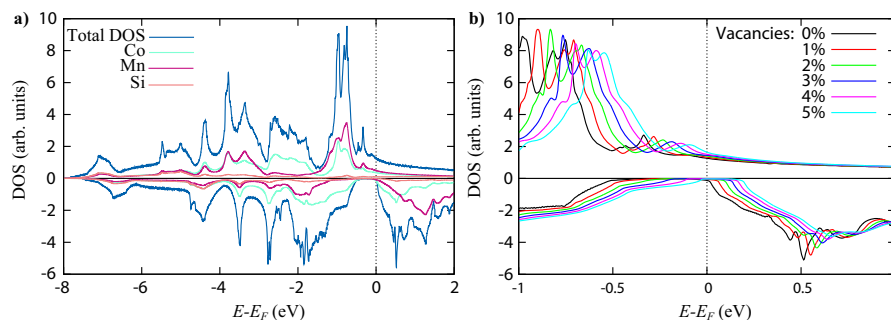


Figure 1. Spin-resolved DOS of Co_2MnSi , a) for the perfect L_{21} phase (with partial contributions of Co, Mn and Si atoms), b) near the Fermi level E_F , as a function of the percentage of vacancies x . Upper and lower panels respectively correspond to majority and minority spin electrons.

3. Results

3.1. Influence of vacancies on the static magnetic properties

The density of states (DOS) of the perfectly ordered L2₁ phase of Co₂MnSi is plotted on Fig. 1a. We found a ferromagnetic half-metallic behaviour, in agreement with previous results from the literature, with a total (spin+orbital) magnetic moment M_{tot} of $4.94 \mu_B$ per unit cell. In Fig. 1b, the DOS is plotted at energies near the Fermi level, as a function of the atom vacancy concentration in the atomic sites. Vacancies may induce impurity states at the low energy side of the minority spin band-gap. The half-metallic character of Co₂MnSi is however preserved, whatever the percentage of atom vacancies we considered, but the minority spin band gap is considerably narrowed by vacancy states or by the shift of electronic states, in particular for the highest contents of these defects: this band gap decreases from 0.43 eV for the perfect crystal to 0.17 eV with 5% of vacancies on each atomic site. In Fig. 2a we can see that the total magnetic moment of the unit cell decreases linearly from about $5 \mu_B$ without vacancies to $4.1 \mu_B$ with 5% of vacancies per atomic site. It should be noted that the value of M_{tot} decreases because magnetic atoms are removed from the crystal, but also because the magnetic atoms which are still present in the crystal have a smaller magnetic moment than in perfect Co₂MnSi, due to the vicinity of vacancies: the magnetic moment decreases from $2.89 \mu_B$ to $2.76 \mu_B$ for Mn atoms and from $1.05 \mu_B$ to $0.80 \mu_B$ for Co atoms, when the vacancy concentration on each atomic site goes from 0 to 5%. This reduction of the magnetic moments is due to a reorganisation of the electron density near vacancies, which is different for majority and minority spins.

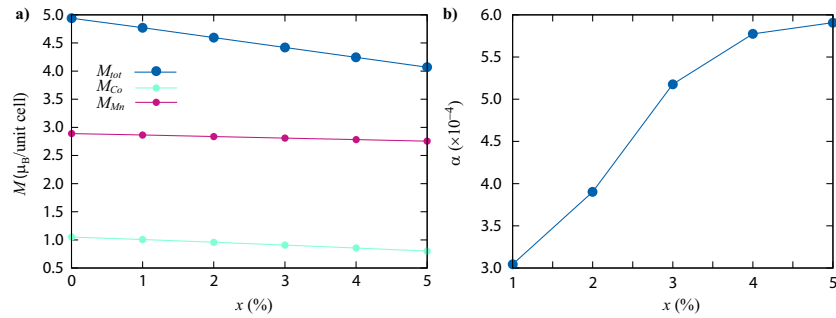


Figure 2. a) Total magnetic moment M_{tot} /unit cell of Co₂MnSi as a function of the percentage of vacancies x , b): α of Co₂MnSi as a function of the percentage of vacancies x .

3.2. Influence of vacancies on the Gilbert damping parameter

The Gilbert damping parameter α is plotted on Fig. 2b as a function of the percentage of atom vacancies x . It is worth noting that since the linear response method cannot calculate α for a totally ordered alloy at 0 K, the Gilbert damping parameter of the perfect L2₁ phase ($x = 0$) is not reported here. The Gilbert damping parameter α increases almost linearly from 3×10^{-4} to 6×10^{-4} when x increases from 1 to 5%. The variation of α can often be connected to changes in the electronic structure of the crystal. The total DOS at the Fermi level Z_F is usually considered as a measurement of the number of channels available for magnetic relaxation. However, below 5% of atom vacancies in Co₂MnSi, there are no major changes in the DOS at the Fermi level, and we must assign the modifications of α induced by atom vacancies to another cause. Kambersky proposed, in order to quantitatively rationalize α , the two following contributions [20]: $\alpha_{sf} = \frac{\pi\gamma\hbar^2}{\mu_0 M} Z_F \frac{(g-2)^2}{\tau}$ and $\alpha_o = \frac{\pi\gamma}{\mu_0 M} Z_F \lambda_{SO} (g-2)^2 \tau$, where α_{sf} is the spin-flip scattering contributions and α_o describes the ordinary scattering. In these equations, γ is the gyromagnetic ratio, M the saturation magnetization, λ_{SO} the spin-orbit coupling parameter, g

the Landé factor and τ the electron scattering time. Relying on this model we can first conclude that the decrease of the total magnetic moment M_{tot} with vacancies (which, in this case is totally proportional to the saturation magnetization since we did not find changes of the unit cell volume induced by vacancies), contribute to an increase of the total magnetic damping α . We can also postulate that atom vacancies are responsible for an increase of the total damping via ordinary and spin-flip scattering, that can be attributed to a lowering of the electron scattering time and/or to an increase of the spin-orbit coupling parameter.

4. Conclusions

We have shown that the presence of vacancies in the L2₁ phase of Co₂MnSi causes a reduction of the total magnetic moment M_{tot} and a reduction of the minority spin band-gap that can be directly related to the increase of the Gilbert damping parameter. This first-principles study of the modifications of the properties of this alloy induced by atoms vacancies could help experimentalists for the interpretation of the physical properties measured on real (imperfect) samples.

Acknowledgments

This work was granted access to the HPC resources of CALMIP supercomputing center under the allocation p1252 (2014-2016).

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