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We present an *ab initio* study of the influence of the tetragonal distortion, on the static and dynamic (Gilbert damping parameter) magnetic properties of a Co_2MnSi crystal. This tetragonal distortion can for instance be due to strain, when Co_2MnSi is grown on a substrate with a small lattice mismatch. Using fully relativistic Korringa-Kohn-Rostoker (KKR) calculations, in conjunction with the coherent potential approximation (CPA) to describe atomic disorder and the linear response formalism to compute the Gilbert damping parameter, we show that a tetragonal distortion can substantially change the properties of Co_2MnSi, in a way which depends on the kind of atomic disorder. [http://dx.doi.org/10.1063/1.4974525]

I. INTRODUCTION

The full-Heusler alloy Co_2MnSi has recently been a subject of intense research activity in the spintronics community. Many theoretical studies have highlighted the half-metallic behavior[1–3] and the very low Gilbert damping parameter (lower than 1×10^{-3})[4] of the perfectly ordered phase of this alloy. These properties, with its high measured Curie temperature of 985 K,[5] make this material a perfect candidate for being used in spintronic applications.

Unfortunately, experimental measurements have shown less impressive magnetic properties than expected from numerical studies: apart from recent measurements reporting a spin-polarization at the Fermi level of 93%[6] or a damping parameter of 1.5×10^{-4},[7] most of the experimental results only found values of the spin-polarization around 50-60%[8–11] and α is in general around 4×10^{-3},[12] more than 10 times higher than the calculated values.

The presence of crystalline defects in the samples was put forward to explain the qualitative difference between measured and calculated properties. Neutron diffraction experiments on thin films confirmed the presence of atomic disorder with mainly Co/Mn swaps.[13,14] Theoretical studies have examined the effects of defects on the static magnetic properties.[2] The torque correlation model (TCM) was used in 2015 to study the impact of atomic disorder on the Gilbert damping parameter for the fully disordered A2 and B2 phases of cubic Co_2MnSi,[3] but a disorder resulting from Co/Mn swaps ($D0_3$-like disorder) has not been considered while it was detected experimentally. Moreover, other defects, like tetragonal deformations, may contribute to the reduction of the spin-polarization at the Fermi level E_F and to the increase of α.

In this paper, we use first-principles methods to calculate, for four crystal phases (nearly-$L2_1$, B2, $D0_3$, A2) of Co_2MnSi, the influence on the static magnetic properties and Gilbert damping parameter of a tetragonal distortion, which may be due to the epitaxial growth of this alloy on a substrate with a small lattice mismatch.

II. CALCULATION DETAILS

All the results presented here were obtained using the SPR-KKR package.[15] Based on the KKR multiple scattering formalism, this code enables to calculate the one-electron Green's function of

defective crystals, describing atomic disorder with the coherent potential approximation (CPA).[16] The main static properties of the system (ground states energy, magnetic moments, density of states) are directly accessible from the calculated Green's function. Moreover, a parameter-free and fully *ab initio* method based on the linear response formalism[17] was implemented to extract the Gilbert damping parameter from the Green's function.

The crystal structure of Co_2MnSi in its most ordered $L2_1$ phase is described by the space groupe $Fm\bar{3}m$, where the Co, Mn and Si atoms occupy respectively the 8c, 4a and 4b Wyckoff positions. In this paper we have also considered: the B2 phase, where Mn and Si atoms are randomly distributed on the 4a and 4b atomic sites; the $D0_3$ phase, where Co and Mn atoms are randomly distributed on the 8c and 4a sites; and the A2 phase where the three atomic species are randomly shared between all the atomic sites.

Since the Gilbert damping parameter cannot be calculated at $T = 0$ K with the linear response formalism for a perfectly ordered phase, the results are not presented for a perfectly ordered $L2_1$, but for a nearly $L2_1$ phase containing a 2% amount of B2-like disorder. We have checked that no significant differences between the $L2_1$ and the nearly $L2_1$ phases were found for the static magnetic properties.

All the calculations were performed with the local spin-density approximation (LSDA) exchange-correlation potential of Vosko, Wilk and Nusair[18] with the fully-relativistic mode. We sampled the irreducible part of 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 for the cubic phase was made and the minimum value of the ground state energy was found for $a_0 = 5.48$ Å. To account for the tetragonal distortions, we constrained the lattice parameters $a_{\parallel} = a_{[100]} = a_{[010]}$ of the tetragonally distorted unit cell of Co_2MnSi to values which can deviate from the calculated lattice constant a_0 of cubic Co_2MnSi: $-5\% \leq \varepsilon_{\parallel} = \frac{a_{\parallel} - a_0}{a_0} \leq 5\%$, where $\varepsilon_{\parallel}$ is the in-plane strain. Then, we calculated the equilibrium lattice parameter $a_{\perp} = a_{[001]}$ by minimizing the total energy. The ratio $a_{\perp}/a_{\parallel}$ decreases almost linearly between 1.12 and 0.91 when $\varepsilon_{\parallel}$ varies from -5% to +5%. These values were calculated for the $L2_1$ phase and were kept for the B2, $D0_3$ and A2 phases.

III. RESULTS

The magnetization (M) of Co_2MnSi is plotted on Fig. 1.a, as a function of $\varepsilon_{\parallel}$ and for the different phases of the crystal. Even without compression, chemical disorder causes large variations of the magnetization, especially for disorders involving Co/Mn swaps like in the $D0_3$ or the A2 phases. It goes from $\approx 120\ \mu_B.nm^{-3}$ for the nearly $L2_1$ and the B2 phases to respectively $\approx 65\ \mu_B.nm^{-3}$ and $\approx 85\ \mu_B.nm^{-3}$ for the $D0_3$ and the A2 phases. The effect of the tetragonal deformation generally tends to reduce even more the magnetization. It decreases for example from $\approx 120\ \mu_B.nm^{-3}$ to $\approx 100\ \mu_B.nm^{-3}$ for $\varepsilon_{\parallel} = -5\%$ for the nearly $L2_1$ phase, mostly because of a decrease of the spin magnetic moment of the Co atoms. For the $D0_3$ phase, the magnetization goes from $\approx 65\ \mu_B.nm^{-3}$ ($\varepsilon_{\parallel} = 0$) to $\approx 20\ \mu_B.nm^{-3}$ ($\varepsilon_{\parallel} = -5\%$), this decrease being due to the decrease of the spin magnetic moment of the Co and Mn atoms in 8c sites. For the A2 phase, the decrease of the magnetization resulting from a compression is due to a decrease of the spin magnetic moments of all the chemical species.

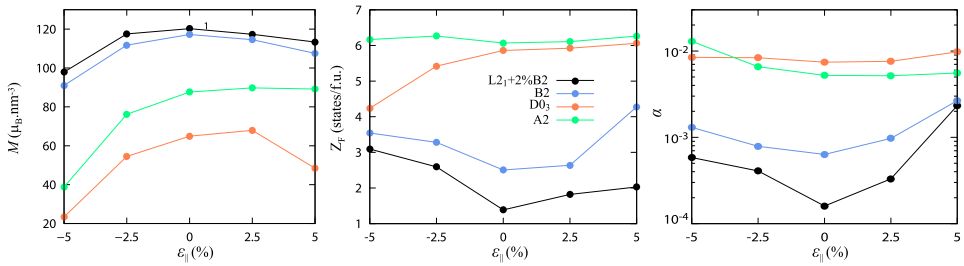

FIG. 1. Impact of the tetragonal distortion on the properties of the 4 phases of Co_2MnSi: a) on the magnetization M, b) on the total density of states at the Fermi level Z_F and c) on the Gilbert damping parameter α.

The total density of states (DOS) at the Fermi level Z_F is plotted on Fig. 1.b. As previously explained, the cubic nearly-$L2_1$ phase being half-metallic, the DOS at E_F is only due to majority spin electrons when $\varepsilon_{\parallel} = 0$, and increases when $\varepsilon_{\parallel} \neq 0$. The half-metallicity of Co_2MnSi is destroyed both by chemical disorder and by tetragonal distortions. Electron states on both sides of the minority spin band gap of the $L2_1$ phase being mainly built from Co d orbitals, disorder-induced modifications of Z_F for cubic crystals ($\varepsilon_{\parallel} = 0$) will be more important for the disordered phases that change the chemical species in the first coordination shell of Co atoms (A2 and $D0_3$ disorders). This explains why Z_F is higher for disordered cubic crystals (in particular for the A2 and $D0_3$ phases) than for the $L2_1$ cubic phase. For non-cubic crystals, the tetragonal distortion lifts the degeneracy between the two e_g and the 3 t_{2g} Co atom orbitals. The minority spin ${d_z}^2$ orbital of Co atoms, which was unoccupied for the cubic crystal, becomes partly occupied when $\varepsilon_{\parallel} < 0$. Conversely, when $\varepsilon_{\parallel} > 0$, the Co ${d_z}^2$ orbital is shifted towards higher energies while the Co $d_{x^2-y^2}$ becomes partly occupied. This explains why Z_F is higher for tetragonally distorted ($\varepsilon_{\parallel} \neq 0$) ordered $L2_1$ crystals than for the cubic ($\varepsilon_{\parallel} = 0$) ordered $L2_1$ crystal (we checked this last point by calculating partial DOS-curves for tetragonally distorted crystals in the $L2_1$ phase, with the code Wien2k[19]). The variations of Z_F as a function of $\varepsilon_{\parallel}$ are stronger for the nearly-$L2_1$, the B2 and the $D0_3$ phases.

A quick analysis of Fig. 1.c shows that any biaxial compression or tension increases the value of α. Except for the A2 phase, this increase is generally higher for $\varepsilon_{\parallel} = 5\%$ than for $\varepsilon_{\parallel} = -5\%$. The effects of the tetragonal distortion are more important for the nearly ordered phase ($L2_1$+2%B2) for which α is 15 times higher for $\varepsilon_{\parallel} = 5\%$ than for the cubic crystal; they are also rather important for the B2 phase (α is more than 4 times higher for $\varepsilon_{\parallel} = 5\%$), moderate for the A2 phase (α is 2.5 times higher for $\varepsilon_{\parallel} = -5\%$), and negligible for the $D0_3$ phase.

The comparison of the different panels of Fig. 1 shows that the increase of the Gilbert damping parameter of a strained disordered layer (with respect to the value calculated for the cubic nearly ordered phase), is due both to the tetragonal distortion and to the alloy disorder when Co_2MnSi is in the B2 phase, but mostly to the alloy disorder when it is in the A2 or in the $D0_3$ phases.

To understand the origin of these variations of α, we used an analytical model proposed by Kamberský, based on the two following contributions:[20] $\alpha_{sf} = \frac{\pi\gamma\hbar^2}{\mu_0 M} Z_F \frac{(g-2)^2}{\tau}$ and $\alpha_o = \frac{\pi\gamma}{\mu_0 M} Z_F \lambda_{SO}^2 (g-2)^2 \tau$, where α_{sf} accounts for the spin-flip scattering contributions and α_o describes the ordinary scattering. In these equations, γ is the gyromagnetic ratio, λ_{SO} the spin-orbit coupling parameter, g the Landé factor and τ the electron scattering time. M and Z_F have the same meaning than before. The variations of α are roughly the same as those of Z_F for the nearly $L2_1$ and the B2 phases: Z_F can be considered as a measure of the number of available relaxation channels and if Z_F is high, the magnetization precession will relax faster. For the $D0_3$ and the A2 cases, we also have to consider the high variations of the magnetization to understand the variations of α ($\alpha \propto \frac{1}{M}$ in the Kamberský model). For the $D0_3$ phase, Z_F and M both decrease with in-plane compression, balancing each other with nearly constant values of α. For the A2 phase, the DOS at E_F does not change with tetragonal distortions, but the magnetization decreases with compression, resulting in an increase of α.

IV. CONCLUSION

We have shown that tetragonal distortions and alloy disorder can substantially change the magnetic properties of Co_2MnSi. Tetragonal distortions are responsible for a strong increase of the Gilbert damping parameter for the nearly-$L2_1$ or the B2 phases, since they have a very low value of α in the cubic structure. It is thus important to avoid any tetragonal distortions to preserve the lowest possible value of α. In comparison, since they already have a high value of α for the cubic cell, the changes induced by the tetragonal deformation are less critical for the $D0_3$ or A2 phases. The priority must be given to a straight control of atomic disorder during the growth of samples, in order to avoid these last phases. The effects of tetragonal distortion and alloy disorder on the physical properties of Co_2MnSi could be analyzed experimentally by performing photoemission spectroscopy (to measure Z_F), magnetometry (to measure M) and ferromagnetic resonance experiments (to measure α) on thin Co_2MnSi layers strained on substrates with different values of the lattice mismatch, and in which alloy disorder could be changed, for instance by irradiation with light ions.[21]

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