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Volume expansion contribution to the magnetism of atomically disordered intermetallic alloys

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The origin of magnetism in atomically disordered transition-metal–nonmagnetic (i.e., FeAl) alloys has been investigated by dichroism and diffraction measurements at high pressure and by band structure calculations. The results show that, in contrast to earlier studies, besides the effects of the local environment of the magnetic ions, disorder-induced lattice changes play a key role in the magnetic properties of these systems. We demonstrate experimentally and theoretically that about 35–45% of the magnetic moment of $Fe_{60}Al_{40}$ alloys arises from lattice expansion effects induced during the disordering process. Such large effects in $Fe_{60}Al_{40}$ could actually be related to the moment-volume instability observed in these alloys.

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I. INTRODUCTION

Transition metal (TM) intermetallics are known to exhibit remarkable functional magnetic properties, ranging from soft FeNi alloys to hard magnetic materials, such as $SmCo_5$.[1] Other intermetallic alloys are more appealing due to their structural properties, e.g., TM aluminides, which show low density, high strength, and good corrosion resistance.[2] This type of alloy often displays unique magnetic properties. For example, the room temperature magnetic moment of *ordered* iron aluminides ($Fe_{1-x}Al_x$) decreases slowly with increasing Al content, consistent with dilution models, up to $x=0.2$. With further dilution the magnetic moment decreases more rapidly, becoming zero for alloys with $x \geqslant 0.35$ of Al.[3] At low temperatures many of these alloys usually exhibit spin-glass properties.[4] Contrarily, *disordered* $Fe_{1-x}Al_x$ alloys are ferromagnetic at room temperature even for alloys with $x > 0.35$.[3,5–15] Similar effects of the disorder on the magnetic properties have been found in many other TM intermetallics, such as CoZr, CoAl, CoGa, CoV, NiSn, FeGe, FePt, and FeV.[16–18] Experimentally, the influence of structural disorder on the magnetic properties has been evidenced, for example, in FeAl, in different types of microstructures such as cold worked single crystals,[9,14] quenched or cold worked polycrystalline materials,[6,7,11] or ball milled and mechanically alloyed nanoparticles.[3,8,10,12,13,15] Moreover, these unusual magnetic properties have led to the possibility of separating the magnetic properties of grain boundaries (*disordered*) from intragrain (*ordered*) properties in ball milled FeAl by the appropriate material processing.[15]

From a theoretical point of view, the magnetism of diluted and disordered TM intermetallic alloys has been traditionally explained by the local *environment model*.[5,19] In this model the magnetic moment of a given TM atom depends on the number of nearest-neighbor TM atoms: (i) either the TM atoms have their full moment when surrounded by a given minimum number of TM neighbors and zero otherwise[6,7,19] or (ii) the moment progressively decreases with reducing the number of TM nearest neighbors below a critical number.[5,8] Using this simple model, the effect of Al substitution and disorder in, e.g., FeAl, can be qualitatively explained.[5–8,19] However, usually no quantitative agreement can be reached[5–8,19–21] and other effects have been proposed as possible explanations for the observed discrepancies. These include antiferromagnetic interactions,[20] next-nearest neighbors or higher order contributions,[5,6,8,18,19] slow decay of the moment away from fully magnetic atoms,[9] or other more complex variations based on Fe-Fe exchange interactions mediated by the nonmagnetic ion.[21] To improve the theoretical understanding of the effects of nonmagnetic ion substitution and disorder, electronic band structure calculations have been performed in many TM intermetallics and, particularly, in FeAl.[22–27] In ordered alloys the reduction of magnetic moment with nonmagnetic ions dilution is satisfactorily explained.[22–27] The effect of disorder has been less investigated, although an enhancement of the magnetic moment with disorder has also been established.[22–24] However, there are certain discrepancies in the equilibrium lattice parameters and the magnetic moments between the theoretical and experimental results.

It is noteworthy that, experimentally, a sizable lattice expansion (or contraction) ($\Delta a_o / a_o \sim \pm 1\%$, where a_o is the lattice parameter) is typically observed in many TM intermetallics subjected to ball milling (e.g., FeAl, CoZr, FeGe, and

CoAl among many others[8,10,12,13,15,28]). Similarly, it is well known that quenching or cold work can also induce local changes in the lattice parameter.[7,11] Taking into account that variations in the distance between TM metals atoms have profound effects on the magnetism,[29] it was actually argued that the origin of the magnetic interactions in disordered TM intermetallics may not arise solely from nearest-neighbors magnetism (i.e., local environment model) but also from changes in the band structure of the material induced by Δa_o.[10] Although experimental evidence of a possible correlation between Δa_o and the magnetic moment has been presented,[10–12] from the theoretical point of view, the effect of Δa_o on the magnetic properties of disordered TM intermetallics has been largely overlooked. Actually, in band structure calculations of disordered TM intermetallics an expansion of the lattice parameter is also found.[22,23,25] However, only recently, indications from band structure calculations that Δa_o could play a role in the magnetic moment of disordered TM intermetallics have been reported.[24] Nonetheless, experimentally, the problem remains on how to separate disorder effects from Δa_o effects. One possibility would be to reduce a_o by deformation without altering the disorder. For such a purpose, ball milled FeAl is an excellent candidate, since it shows $\Delta a_o/a_o$ on the order of 1% and its large hardness[30] ensures a high elastic limit. Unfortunately, measurements of the magnetic moment in pressures large enough to significantly change a_o are not straightforward. However, it has been demonstrated that x-ray magnetic circular dichroism (XMCD) could be used for such purposes.[31] Although this technique has been applied to investigate magnetism in single crystals and foils,[32] it has seldom been used to study powdered samples so far.[33,34]

In this article we present the study of the evolution of the magnetic moment of a ball milled $Fe_{60}Al_{40}$ alloy with applied pressure using XMCD, with the aim to separate the effects of disorder from those of lattice expansion on the magnetic properties. Experimental and theoretical results indicate that, contrary to previous reports, the milling induced lattice expansion plays an important role in the magnetic properties of this type of alloys. For example, in $Fe_{60}Al_{40}$, the Δa_o effect contributes about 35–45% to the magnetic moment of this alloy.

II. EXPERIMENTAL

Samples were prepared by ball milling atomized $Fe_{60}Al_{40}$ alloy powders for 32 h, under Ar atmosphere, using agate vials and zirconia balls, with a ball-to-powder ratio of 4:1.[10]

X-ray diffraction (XRD) experiments under pressure were performed on the as-milled powders on beamline ID9A of the European Synchrotron Radiation Facility (ESRF, Grenoble) using monochromatic radiation of $\lambda = 0.4175$ Å. Diffraction images were recorded with a MAR345 image plate system and then integrated using the FIT2D software,[35] to yield intensity versus 2θ diagrams. A diamond anvil cell (DAC) was used for pressure generation with nitrogen as a pressure medium to provide nearly hydrostatic conditions. The experiment was performed at room temperature using different pressures up to 12 GPa. The applied pressure was estimated by the ruby luminescence method.[36]

The high-pressure XMCD experiments at the Fe *K* edge (7112 eV) (Ref. 37) were carried out on the energy dispersive x-ray absorption beamline ID24 (Refs. 34 and 38) at ESRF. The sample consisted of plateletlike grains of milled $Fe_{60}Al_{40}$ (5–10 μm in diameter) placed between the plates of a CuBe DAC in a silicon oil pressure transmitting medium. Spectra were taken for both right and left polarization of the beam. Further, in order to improve the signal-to-noise ratio, a large number of spectra were taken at each polarization and averaged. For each pressure, in order to normalize the XMCD signal to account for the inhomogeneous thickness of the grains and for the thickness reduction under pressure, the absorption spectra were recorded simultaneously to the XMCD spectra. The normalized XMCD spectra are given as the intensity of the XMCD spectrum divided by the edge jump of the absorption spectrum. The normalized XMCD spectrum was finally integrated over the 7100–7125 eV range to obtain a "normalized integrated intensity," which is proportional to the magnetic moment of the sample.[39]

Magnetization measurements under pressure up to 1.4 GPa were performed at room temperature in magnetic fields up to 15 kOe using a vibrating sample magnetometer (VSM). A miniature CuBe container with a mixture of mineral oil and kerosene as pressure-transmitting medium was used for the experiment.

Electronic band structure calculations of ordered (*B*2) and disordered (*A*2) $Fe_{62}Al_{38}$ alloys were obtained from self-consistent electronic calculations using a tight binding linear muffin tin orbital (TB-LMTO).[40] To obtain the magnetic moment of the alloy, the von Barth and Hedin parametrization[41] for the local spin-density approximation was used, which is a good approximation for these calculations.[22] Note that other approaches, such as the generalized gradient approximation (GGA), have been successfully used to study similar intermetallic alloys.[42] However, these approaches have failed to reproduce the ground state in the FeAl system.[43] The *B*2 ordered and *A*2 disordered structures have been built following Schmid and Binder.[44] In order to make a good approximation of the disorder, the average of five different *A*2 supercells has been used, each one containing 32 atoms. The presented values correspond to the mean value of the five supercells.

III. RESULTS

A. Experiment

The as-atomized $Fe_{60}Al_{40}$ powder exhibits an ordered *B*2 structure with a lattice parameter of $a_o(B2) = 0.28980(2)$ nm. During ball milling the alloy disorders, the order parameter evolving from a fully ordered $S = 0.80$ before milling to an almost completely disordered $S = 0.14$ after the milling,[10] transforming into an *A*2 structure with a lattice parameter of $a_o(A2) = 0.2917(1)$ nm. Hence, apart from the structural disorder, milling also induces a lattice expansion of about $\Delta a_o/a_o \sim 0.7\%$. The disordered *A*2 alloy is ferromagnetic with a saturation magnetization of $M_S \sim 75$ emu/g, while

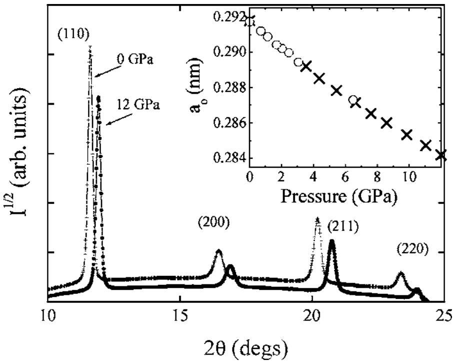

FIG. 1. XRD spectra at 0 GPa (+) and 12 GPa (●) applied pressures, for a ball milled $Fe_{60}Al_{40}$ alloy. Shown in the inset is the lattice parameter, a_o, as a function of the applied pressure. Note that the a_o values determined upon increasing (×) and decreasing (○) pressure experiments are plotted together.

the ordered $B2$ one shows virtually no magnetization ($M_S < 0.2$ emu/g).[10]

Shown in Fig. 1 are the XRD patterns of the disordered FeAl alloy at two different pressures. The analysis of the evolution of the XRD spectra with applied pressure shows that $Fe_{60}Al_{40}$ exhibits no phase transitions in the range of pressures used (0–12 GPa). Moreover, the lack of hysteresis, when increasing and decreasing pressure (see Fig. 1 inset), implies that the material remains within the elastic range, as expected from its large hardness. The zero-pressure bulk modulus, B_0, obtained from the pressure dependence of the unit cell volume, $B_0 = 123$ GPa, is consistent with earlier experimental and theoretical estimates for FeAl.[22,45] Notably, the pressure does not change the order parameter of the disordered alloy. As can be seen from Fig. 1, the lattice parameter is reduced about 3% between 0 and 12 GPa.

The saturation magnetization, M_S, of $Fe_{60}Al_{40}$ measured by VSM shows rather small changes with applied pressure up to 1.4 GPa, where maximum changes of M_S of the order of only 3±2% have been observed [see Fig. 2(b), filled symbols], i.e., in the limit of the instrumental resolution. Hence, the results indicate that 1.4 GPa (with about $\Delta a_o/a_o \sim 0.3\%$) induces no significant changes in the magnetism of the alloy.

As can be seen in Fig. 2(a), as the pressure is increased the area of the XMCD spectra decreases, indicating a reduction of the magnetic moment for smaller a_o. When integrating the XMCD spectra for each pressure and plotting it versus a_o [Fig. 2(b), open symbols], it can be clearly observed that the integrated XMCD intensity remains roughly constant until a_o of about 0.29 nm is reached (in agreement with VSM results). When a_o is further reduced (i.e., at larger pressures), a magnetic phase transition is observed, leading to a rapid decrease of the normalized integrated intensity (i.e., the magnetic moment) reaching a value of about 0.65. This indicates that when a_o reaches approximately the one for the ordered sample, up to 35±5% of the magnetic moment of the sample vanishes. Finally, as a_o is further decreased with pressure, no additional significant changes occur in the magnetic moment of the sample. This sharp magnetic transition indicates the existence of a moment-volume instability, similar to the ones predicted (and in some cases observed) in many ordered and disordered intermetallics, e.g., FePt or FeNi.[46] Actually, in $Fe_{50}Al_{50}$ and $Fe_{75}Al_{25}$, similar moment-volume instabilities, exhibiting high and low moment states at different lattice parameters had been predicted by band structure calculations in both ordered and disordered systems,[24,25] but had never been observed experimentally.

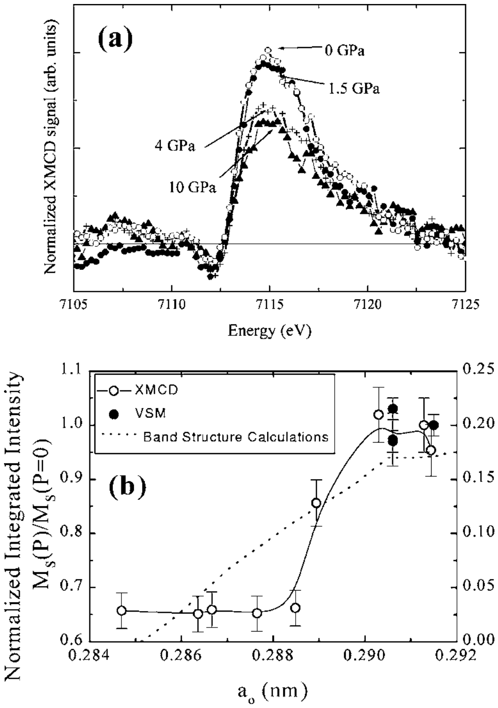

FIG. 2. (a) Pressure dependence of the normalized x-ray magnetic circular dichroism (XMCD) around the Fe K edge for a ball milled $Fe_{60}Al_{40}$ alloy. (b) Normalized XMCD integrated intensity (open symbols) and normalized saturation magnetization (filled symbols) vs the lattice parameter, a_o, for a ball milled $Fe_{60}Al_{40}$ alloy. The dashed line shows the evolution of difference between the magnetic moment of the disordered alloy, μ^{A2}, and the equilibrium magnetic moment of the ordered alloy, $\mu^{B2}[a_o(B2)]$, as a function of the lattice parameter, a_o, for a $Fe_{62}Al_{38}$ alloy. The continuous lines are guides to the eye.

B. Band structure calculations

The calculations give an equilibrium lattice parameter for the ordered phase of 10.8084 atomic units (0.286 nm), a value which underestimates by about 1.5% the experimental value. In the disordered structure the calculated equilibrium lattice parameter underestimates the experimental value by about 1.8%. These results are in agreement with local density approximation calculations in these alloys.[22] Moreover, the calculations give bulk moduli of 186 GPa and 169 GPa for the ordered and disordered structures, following the trend found in these alloys.[22]

The contribution to the enhancement of the total moment ($\Delta\mu_{Tot}$) from lattice expansion ($\Delta\mu_{Vol}$) and from disorder ($\Delta\mu_{Dis}$) can actually be easily separated, $\Delta\mu_{Tot} = \Delta\mu_{Dis} + \Delta\mu_{Vol}$, from the difference between μ of the disordered alloy, $\mu^{A2}[a_o]$, and of the ordered alloy at its equilibrium $a_o(B2)$ lattice parameter, $\mu^{B2}[a_o(B2)]$, as discussed by Apiñaniz.[24] Using the definition in Ref. 24 for $\Delta\mu_{\mathrm{Tot}}$, $\Delta\mu_{\mathrm{Dis}}$, and $\Delta\mu_{\mathrm{Vol}}$, we obtain that the contribution of Δa_o to the total magnetic moment, $\Delta\mu_{\mathrm{Vol}}/\Delta\mu_{\mathrm{Tot}}$, is about 45±10%. As expected, this value is intermediate between the ones obtained for $Fe_{75}Al_{25}$ and $Fe_{50}Al_{50}$.[24] Moreover, as can be seen in Fig. 2, where $\mu^{A2}[a_o]-\mu^{B2}[a_o(B2)]$ is plotted, a transition between high and low moment states can be inferred in the same a_o range (note the change of slope around $a_o = 0.291$ nm) as the one found experimentally, although somewhat broader. It is noteworthy that similar magnetic transitions, although sharper, have been theoretically obtained for ordered $Fe_{75}Al_{25}$ and $Fe_{50}Al_{50}$.[24]

IV. DISCUSSION

To understand the mechanism of the magnetic phase transition, one has to look at the density of states (DOS) of the intermetallic alloy.[22] Actually, Fe atoms surrounded by many nonmagnetic nearest neighbors show an abrupt change of μ with a_o, caused by the presence of a narrow peak in the partial DOS of those Fe atoms in the neighborhood of the Fermi level, which crosses the Fermi level with variations of a_o.[22] However, Fe atoms surrounded by many Fe nearest neighbors exhibit a monotonous and smooth variation of μ. The DOS indicates that at large a_o there is a weak hybridization between Fe and Al. However, with decreasing lattice parameter there is a strengthening of the hybridization, which gives rise to charge transfer from the majority to the minority spin subbands, in turn, causing the decrease of the magnetic moment with reducing a_o. For lattice parameters above the equilibrium one the narrow subpeak in the DOS close to the Fermi level is completely full. As the lattice parameter is decreased, this peak in the majority spin subband empties almost completely, while concomitantly the minority spin subband fills. This causes the difference between the two subbands to decrease and therefore the magnetic moment decreases abruptly.

Hence, the results from the band structure calculations confirm the experimental finding that Δa_o in disordered TM-nonmagnetic alloys plays an important role in their magnetism. Note that although for $Fe_{60}Al_{40}$ probably the moment-volume instability may enhance this volume expansion contribution to the magnetism, such Δa_o effect should be present in many other intermetallic systems as a result of changes in the magnetic moment with increasing a_o, due to a stronger polarization of the d bands or a localization of the electrons in the TM ions. The exact relative contribution of each factor depends on the actual band structure of the alloy and hence on the elements involved and the composition of the alloy, in particular, the presence of sharp DOS peaks close to the Fermi level may enhance the effect. These results suggest that the effect of disorder-induced Δa_o should be taken into account when discussing the magnetic properties of ball milled or deformed alloys, not only in TM intermetallics but probably also in other materials.

V. CONCLUSIONS

In conclusion, the origin of the magnetic moment of atomically disordered transition-metal–nonmagnetic intermetallics has been studied experimentally and by band structure calculations. XMCD measurements under pressure in ball milled $Fe_{60}Al_{40}$ (disordered) alloys show that magnetic moment decreases as the lattice parameter is reduced. The theoretical magnetic moment obtained from the electronic band structure exhibits a similar trend. These results demonstrate that the magnetism in this kind of system arises both from the atomic disorder and the disorder-induced lattice expansion. This is in contrast to previous studies where only near-neighbor effects were considered to explain the magnetic behavior of similar alloys. In the case of disordered $Fe_{60}Al_{40}$, experimentally the contribution of disorder and lattice expansion account for 65% and 35% of the magnetism of the alloy, respectively.

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