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Magnetic splitting in x-ray photoelectron spectroscopy Cr L spectra of Fe₂CrAl, Co₂CrAl and Cu₂CrAl

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Abstract

We have investigated various Cr-based Heusler alloys using core-level x-ray photoelectron spectroscopy (XPS). Of special interest are the 2p XPS lines, which always exhibit magnetic splitting in the case of the existence of a well-defined local magnetic moment at the transition metal site. The Cr 2p XP spectra, however, do not exhibit this exchange splitting for the nonmagnetic Cu₂CrAl sample and for Fe₂CrAl or Co₂CrAl alloys with a magnetic moment at the Cr sites of about 1.6 μ_B . This behaviour is discussed here.

1. Introduction

Heusler-type alloys are ternary L₂₁ compounds of the form X₂YZ, where X and Y are two different transition metals and Z is a nonmagnetic metal or a nonmetallic element. These alloys have been widely investigated and it is primarily their magnetic properties that have drawn so much attention to these materials [1]. Most of these alloys are magnetically ordered; their magnetism is due to one or more 3d elements occupying the X or Y sites, or both. The origin of the ferromagnetism and the problem of the local magnetic moment—that is, localized behaviour in some aspects of itinerant d electrons—constitute a challenging problem for the Heusler alloys. In Heusler alloys of the X₂MnZ type the magnetic moment of Mn atoms is about 4 μ_B ; it is reported in references [2–5] to be independent of the nature of the X element and the Z element, and behaves like localized Mn moments in an insulator [6].

The magnetic behaviour of the X₂CoZ alloys contrasts sharply with that of most of the Mn Heusler alloys; the itinerant character of the 3d electrons and the strong dependence of the magnetic moment μ_{Co} of Co atoms on the partner element X and Z are almost always observed. The decrease of the magnetic moment μ_{Co} is explained in reference [6] as being a result of a reduced exchange splitting due to hybridization and charge transfer of the 3d electrons and the s, p, d electrons of the Z nonmagnetic partner element. The problem of localized against delocalized screening of the 3d valence electrons of the transition element can also strongly influence the core-level photoelectron spectra as was elaborated, e.g., in reference [7].

Recently we observed the exchange splitting of the Mn 2p_{3/2} lines which gives evidence of the existence of well-defined magnetic moments at the Mn sites in the Mn-based Heusler

alloys [8, 9]. A clear correlation of the $2p_{3/2}$ splittings observed in the Mn-based Heusler alloys allowed us to consider the Mn spectrum as ‘atomiclike’ [10]. This is in qualitative agreement with the description of local magnetic moments in Mn [5, 11]. We found that the splitting of the Mn $2p_{3/2}$ level is directly correlated with the value of the local magnetic moment at the Mn site [9, 13].

We also observed the splitting of Cr 2p core levels in a number of ternary ACr_2X_4 ($A = Cd, Hg, Cu, Fe, Mn; X = S, Se$) magnetic compounds, which indicates the localized character of the magnetic moments for Cr in a $3d^3$ configuration [12]. The size of the splitting of the Cr 2p levels for ACr_2X_4 samples indicates that the value of the local magnetic moment of the chromium ions in a $3d^3$ configuration is comparable to that of Mn ions, although they may exhibit completely different macroscopic magnetic ordering. The local magnetic moment of about $3 \mu_B$ per Cr ion leads to a splitting of about 1 eV [12].

In this work we study the 3d XP spectra of various Cr-based Heusler alloys, having the nonmagnetic ground state (Cu_2CrAl) or a magnetic moment of $1.67 \mu_B$ /formula unit for Fe_2CrAl and $1.55 \mu_B$ /formula unit for Co_2CrAl [6]. We suggest why the magnetic splitting in Cr 2p XP spectra is not visible. The results obtained here fully support the assertion that 2p XP spectroscopy performed on a transition metal is an effective technique to use to achieve an understanding of the localized magnetic moment formation either in the alloy or in the compound.

2. Experimental details

The X_2CrAl samples, where $X = Fe, Co$ and Cu , were prepared by arc melting the constituent metals on a water-cooled copper hearth in a high-purity argon atmosphere. The phase purity of these compounds was ascertained by means of x-ray Debye–Scherrer diffraction with $Cu K\alpha$ radiation using a SIEMENS D-5000 diffractometer. The x-ray photoelectron spectra were measured using a PHI 5700 spectrometer with an energy resolution of 0.3 eV of the monochromatized $Al K\alpha$ radiation. For Cu_2CrAl we measured the 2p XP spectra with unmonochromatized $Mg K\alpha$ radiation in order to avoid the superposition of core-level intensities with the corresponding Auger Cu LMM peak.

3. Results and discussion

Displayed in figure 1 are Cr 2p XP spectra for different X_2CrAl alloys. Also shown in the figure, for comparison, is the Cr 2p XP spectrum for $CuCr_2Se_4$ single crystal [12]. The spectra are normalized to their maximum. The binding energy of the Cr $2p_{3/2}$ level is about 575 eV. The XPS data for the ionic compound $CuCr_2Se_4$ exhibit a clear exchange splitting of the $Cr2p_{3/2}$ line, which is of about 1 eV [12]. This splitting of the core 2p levels was attributed to the spin polarization of the $3d^3$ states in chromium, which lead to a magnetic moment very close to that obtained experimentally: $\sim 3 \mu_B$. Note, that the Cr $2p_{3/2}$ splitting $\Delta E \sim 1$ eV is in agreement with that obtained experimentally in reference [13]. The $2p_{3/2}$ splitting energy (ΔE) data plotted as ΔE versus μ_{Mn} for a series of different Mn Heusler alloys exhibit a universal linear dependence, which gives for $\mu = 3 \mu_B$ a value of $\Delta E \sim 1$ eV. As shown in figure 1, the Heusler alloys do not exhibit any splitting in the Cr 2p XP spectra; this suggests a nonmagnetic ground state or strongly delocalized Cr d states or both, or that the magnetic moment localized on Cr atoms is not large enough for one to detect the splitting (this is discussed below).

Some change of the magnetic moment of Cr atoms can be explained as a result of different exchange splitting due to hybridization, while the transfer of the 3d electrons and the s, p, d

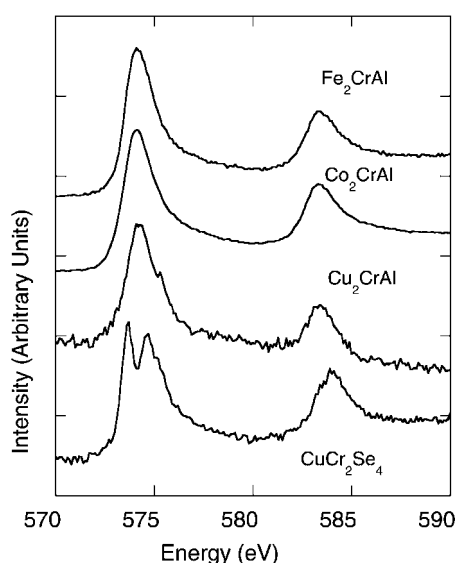


Figure 1. XP Cr $2p_{3/2}$ and $2p_{1/2}$ core-level spectra of the Heusler alloys containing Fe, Co and Cu. For Cu_2CrAl the 2p spectrum is measured with Mg $K\alpha$ radiation to separate out the Cu LMM Auger line; the other spectra are measured with Al $K\alpha$ x-rays. For comparison, we also present the Cr 2p XP spectrum for the ionic compound CuCr_2Se_4 which was published in reference [8].

electrons of Al should be the same for these three alloys. However, it is not clear why Cr is nonmagnetic in Cu_2CrAl and why it has a magnetic moment $\sim 1.6 \mu_B$ in Fe_2CrAl and Co_2CrAl . One reason is a crystal-field (CF) splitting. Cr atoms form a tetrahedron in the crystalline lattice of X_2CrAl . The CF theory predicts for this tetrahedral geometry the e_g state as a ground state. If chromium appears as Cr^{2+} ($3d^4 4s^2$) then both states—lower, e_g , and higher, t_2g —are nonmagnetic due to Hund's rules. Relatively weak hybridization between the Cr and Cu d states does not change the nonmagnetic state of the Cu_2CrAl sample. The hybridization between Cr and Fe or Co d states is much stronger and can lead to the magnetism—even to the nonmagnetic ground state being preferred in a tetrahedral distribution of Cr atoms. As was mentioned, the magnetic splitting of the 2p level can be experimentally observed only for that magnetic element of d type which has a localized magnetic moment larger than $2 \mu_B$ [13]. Therefore, a 2p splitting in Fe_2CrAl or Co_2CrAl is not detected, in spite of the magnetic moment in Cr atoms of $\sim 1.6 \mu_B$.

The $2p_{3/2}$ splittings observed in intermetallic compounds correlate with the local magnetic moments, whereas the 3s splittings do not show such a correlation. In reference [14], the observed 3s XPS peak splittings do not correlate with the Fe magnetic moments in the alloys containing Fe. The Fe 3s peaks of several Fe intermetallics exhibit a splitting of 4.3–4.7 eV, while the measurements of the magnetic susceptibility showed that these compounds are Pauli paramagnets. For the compounds investigated we do not present the 3s XP spectra of Fe and Cr; both display a splitting of ~ 4.5 eV and a small ratio of the satellite to the main-peak intensity (for the Fe 3s XPS lines this ratio is less than 0.2). Probably the satellites in these intermetallic compounds have to be attributed to interband transitions and not to a low-spin component, which might be for some reason quenched in the metallic systems.

In conclusion, we present Cr 2p XP spectra which do not exhibit a splitting, which is characteristic for d elements with localized magnetic moment larger than $2 \mu_B/\text{atom}$. Our

data provide a quick way to show that the local magnetic moments of Cr in XP spectroscopy are very useful in investigating magnetic materials.

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