KLL Auger spectra of 3d transition metals (Cu, Ni) and their alloys

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We present the first high resolution KLL Auger spectra (excited by Cu X-rays) of polycrystalline Cu and Ni metallic samples, in comparison with similar spectra obtained from some binary alloys of these metals. The relative energies and intensities of the $KL_{23}L_{23}$ lines are in a good agreement with the experimental and theoretical data obtained earlier, while in the case of the absolute Auger transition energies considerable deviations occur.

1. Introduction

High energy resolution, X-ray excited, deep core Auger Spectroscopy of surfaces and interfaces of practical interest – such as the surfaces of 3d transition metals – is important for providing possibilities for accurate determination of high energy Auger parameters (applicable for deriving charge transfer and polarization) and for nondestructive depth profiling of subsurface layers. The detailed knowledge of the KLL Auger spectra of Cu and Ni provides important information on the electronic structure of these metals. Earlier experimental studies on X-ray excited Cu KLL transitions [1], performed in a moderate vacuum, showed the presence of a satellite of the main $^1D_2$ line, attributing it to an electron loss contribution.

2. Experimental

Cu and Ni KLL spectra were excited by Cu X-rays from Cu and Ni layers of 10 nm thickness, vacuum evaporated onto Si wafer substrates, as well as from polycrystalline Cu_3Au, $CuAu_3$ and NiFe alloy samples. Following in situ Ar^+ sputter cleaning of the sample surface, measurements of high energy electron spectra were performed using a home built, high luminosity electron spectrometer [2] based on a hemispherical analyzer, with an energy resolution of 1.3 eV. In the high energy range the energy calibration of the spectra is based on the measurement of the Cu 2p lines excited by Cu Kα X-rays [3,4]. The cleanliness of sample surfaces was monitored by Al Kα excited XPS spectra and the vacuum level during measurements was better than 10^{-9} mbar. Evaluating the spectra, Voigtian lineshapes and a modified Tougaard-type background correction ([5], B'=0.1B;C'=0.1C) were used.

3. Results and Discussion

The X-ray induced Cu and Ni KLL Auger spectra excited from thin metallic layers are presented in Figs 1 and 2. From these spectra the presence of the satellites in the case of clean Cu and Ni samples is obvious. In our recent paper [6] we provide evidences that the satellites are similar in these metals and in their alloys and they can be attributed to 3d shake-up processes. Due to the good energy resolution, the $KL_3L_3(^3P_0)$ lines can also be identified in our spectra, in contrast with the previous measurement [2].

The results of the evaluation of our spectra are summarized in Tables 1-4. While the present Cu KLL and Ni KLL relative energies (Tables 1-2) are in a rather good agreement with both the earlier experimental [1] and theoretical [7,8] data, the absolute Auger transition energies differ considerably. As for the relative intensities of the KLL lines (Tables 3-4), the agreement again is remarkable and amongst the available theoretical approaches [8-10] the

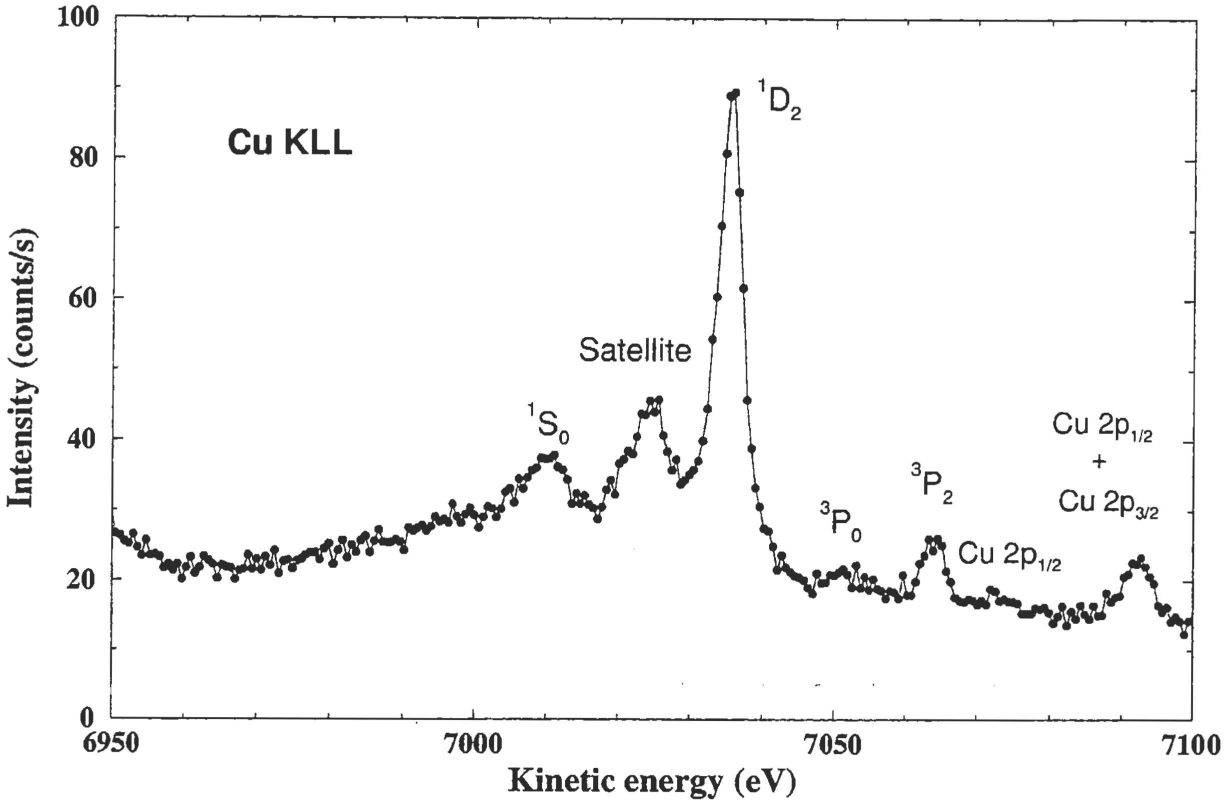

Fig. 1 X-ray excited KLL Auger spectra of a metallic Cu layer of ca 10 nm thickness, vacuum evaporated onto a Si substrate

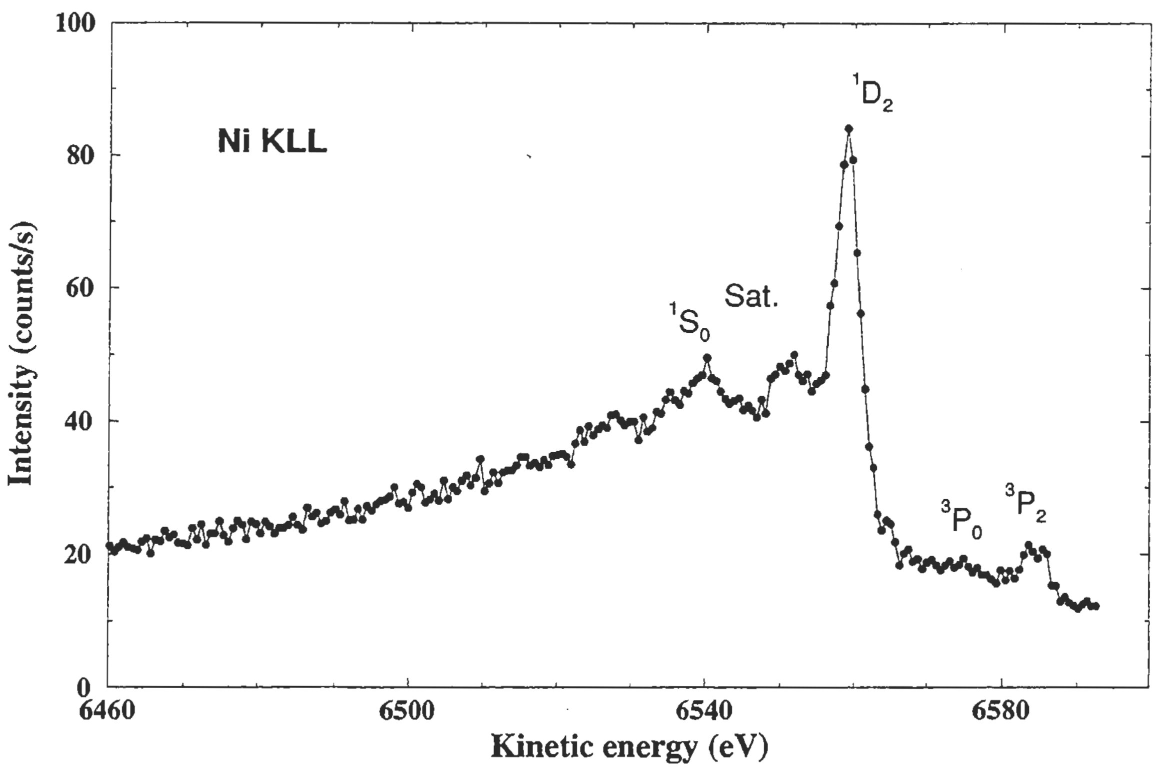

Fig. 2 X-ray excited KLL Auger spectra of a metallic Ni layer of ca 10 nm thickness, vacuum evaporated onto a Si substrate

configuration interaction, intermediate coupling relativistic model of Chen et al [9] seems to be the most successful one. Our results demonstrate that the achieved accuracy of the measurements of the Cu KLL Auger energies makes possible the determination of small alloy-metal shifts of deep core Auger parameters in the case of Cu-Au alloys, contributing to the solution of controversial issues concerning charge transfer in these systems[11].

Table 1

Cu KLL relative energies (eV)

Line	Present work (E)	[1] (E)	[7](T)	[8](T)
Satellite	-11.4(0.7)	-	-	-
$KL_2L_2(^1S_0)$	-25.8(1.3)	-29(0.3)	-24,2	-29
$KL_2L_3(^1D_2)$	0	0	0	0
$KL_3L_3(^3P_0)$	15.9 (2.3)	-	16.3	-
$KL_3L_3(^3P_2)$	28.5 (0.6)	28 (0.3)	26.6	26
$E(KL_2L_3\ ^1D_2)$	7038.3 (0.5)	7034.5 (1.0)	7031.1	-

Table 2

Ni KLL relative energies (eV)

Line	Present work (E)	[7] (T)
Satellite	-7.1 (1.5)	-
$KL_2L_2(^1S_0)$	-19.4 (1.8)	-21.6
$KL_2L_3(^1D_2)$	0	0
$KL_3L_3(^3P_0)$	16.3 (2.3)	14.5
$KL_3L_3(^3P_2)$	25.1(1.0)	24.8
$E(KL_2L_3\ ^1D_2)$	6559.1 (0.5)	6542.1

Table 3

Cu KLL relative intensities

Line	Present work (E)	[1] (E)	[9] (T)	[8] (T)
Satellite	16 (0.4)	-	-	-
$KL_2L_2(^1S_0)$	14 (0.2)	13	9	7
$KL_2L_3(^1D_2)$	100	100	100	100
$KL_3L_3(^3P_0)$	7(0.2)	-	4	-
$KL_3L_3(^3P_2)$	15(0.2)	13	12	14
$I(^3P_2)/I(^3P_0)$	2.1	-	3	-

Table 4

Ni KLL relative intensities (eV)

Line	Present work (E)	[8] (T)	[9] (T)
Satellite	26(0.3)	-	-
$KL_2L_2(^1S_0)$	14 (0.2)	9	10
$KL_2L_3(^1D_2)$	100	100	100
$KL_3L_3(^3P_0)$	5(0.1)	3	3
$KL_3L_3(^3P_2)$	12(0.2)	15	15
$I(^3P_2)/I(^3P_0)$	2.4	5	5

4. Conclusion

The first high resolution X-ray excited KLL Auger spectra of polycrystalline Cu and Ni are presented. A good agreement is obtained between our results and those obtained earlier concerning the relative energies and intensities of the respective Auger lines, while the difference in the case of the absolute Auger transition energies is significant.

5. Acknowledgement

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