

Cr-K β X-ray Emission Spectra in Several Chromium Compounds

Tatsunori Tochio, A.M.Vlaicu, Takashi Ishizuka, Daisuke Osawa,
Yoshiaki Ito and Takeshi Mukoyama

Cr- K β x-ray emission spectra in chromium metal and five chromium compounds were measured by using a double crystal spectrometer with high resolution. Differences in the appearance of K β' and K β'' satellite lines are confirmed in the spectra of the compounds. The origin of K β' and K β'' satellite lines is discussed due to both the number of unpaired electrons and the symmetry of ligands around the chromium atom.

Keywords: K β' and K β'' satellite lines/ exchange interaction/ number of unpaired electrons/symmetry of ligands/ molecular orbital

The K x-ray emission spectra of 3d transition elements have been with great interests for a long time because of their asymmetric shapes or the existence of satellite lines. These features indicate that some processes or interactions play an important role besides single electron transition between the levels of the diagram lines. Although multielectron excitations or multiplet splitting, etc. may be considered as origins of satellite lines, the origins of many satellite lines remain not clarified. Therefore, in order to elucidate the mechanism of their origins (especially of K β' and K β'' satellite lines) the K x-ray emission spectra of chromium in Cr metal, Cr₂O₃, CoCr₂O₄, FeCr₂O₄, K₂CrO₄ and K₂Cr₂O₇ were measured using a double crystal spectrometer with high resolution.

The K β satellite line appears on the low energy side of the K $\beta_{1,3}$ lines which are originated from the single electron transition of 3p→1s. As can be seen from Figure1, the relative

intensity of the K β' satellite line to the K $\beta_{1,3}$ lines for compound with octahedral symmetry is larger than that for compound with tetrahedral symmetry. Tsutsumi suggested that the K β satellite line might be attributed to the exchange interaction between the total spin of 3p electrons s and that of 3d electrons S [1]. The Hamiltonian of this exchange interaction is given by

$$- (J/2)(1+4S \cdot s),$$

where J is the exchange integral. When one electron in the filled 3p shell moves into the vacancy in the 1s shell, this exchange interaction causes the energy splitting of the final states by the energy of DE which is given by

$$\Delta E = J(2S+1),$$

where S is the magnitude of S . The value of ΔE derived from this theory agrees well with the energy difference between the K $\beta_{1,3}$ lines and the K β satellite line in observed

STATES AND STRUCTURES —Atomic and Molecular Physics—

Scope of research

In order to obtain fundamental information on property and the structure of materials, the electronic states of atoms and molecules are investigated in detail using X-ray, synchrotron radiation, ion beam from accelerator and nuclear radiation from radioisotopes. Theoretical analysis of the electronic states and development of new radiation detectors are also performed.



Prof
MUKOYAMA,
Takeshi (D Eng)



Instr
KATANO,
Rintaro (D Eng)



Instr
ITO,
Yoshiaki (D Sc)



Instr
NAKAMATSU,
Hirohide (D Sc)

Guest Res Assoc

Turgut Bastug (D Sc)

Students

YAMAGUCHI, Koichiro (DC)
OSAWA, Daisuke (DC)
SHIGEMI, Akio (DC)
SUZUKI, Chikashi (DC)
TOCHIO, Tatsunori (DC)
MASAOKA, Sei (MC)
ISHIZUKA, Takashi (MC)
NAKANISHI, Yoshikazu (RF)
Vlaicu A. Mihai (RS)

spectra. According to this theory, the relative intensity of $K\beta$ satellite lines to the $K\beta_{1,3}$ line is given by $S/(S+1)$. The number of unpaired electrons is formally three ($S=3/2$) in the compounds with octahedral symmetry, zero ($S=0$) in the compounds with tetrahedral symmetry. Then this theory can account for the larger intensity of the $K\beta'$ lines in the compounds with octahedral symmetry. But it cannot explain the $K\beta''$ satellite line quantitatively and needs some modifications. Some trials to get better agreement by some modifications such as consideration of the effect of spectator hole or plasmon were performed [2][3]. However, some other modifications are still needed to account for the origin of the $K\beta$ satellite line sufficiently.

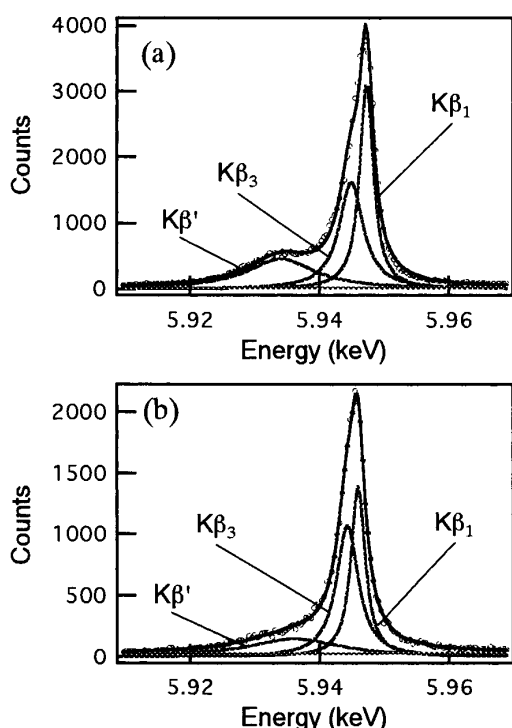


Figure 1. (a): The $K\beta_{1,3}$ and $K\beta'$ spectra of FeCr_2O_4 (octahedral symmetry), (b): The $K\beta_{1,3}$ and $K\beta'$ spectra of $\text{K}_2\text{Cr}_2\text{O}_7$ (tetrahedral symmetry)

The $K\beta''$ satellite lines with the $K\beta_{2,5}$ lines of chromium in FeCr_2O_4 (octahedral symmetry) and $\text{K}_2\text{Cr}_2\text{O}_7$ (tetrahedral symmetry) are shown in figure 2. The $K\beta''$ satellite line appears on the high energy side of the $K\beta_{2,5}$ lines. The $K\beta_2$ line and the $K\beta_5$ line are generated by the single electron transition of $4p \rightarrow 1s$ and $3d \rightarrow 1s$ respectively. It is easily seen that the relative intensity of $K\beta''$ satellite line to the $K\beta_{2,5}$ lines in $\text{K}_2\text{Cr}_2\text{O}_7$ (tetrahedral symmetry) is much larger than that in

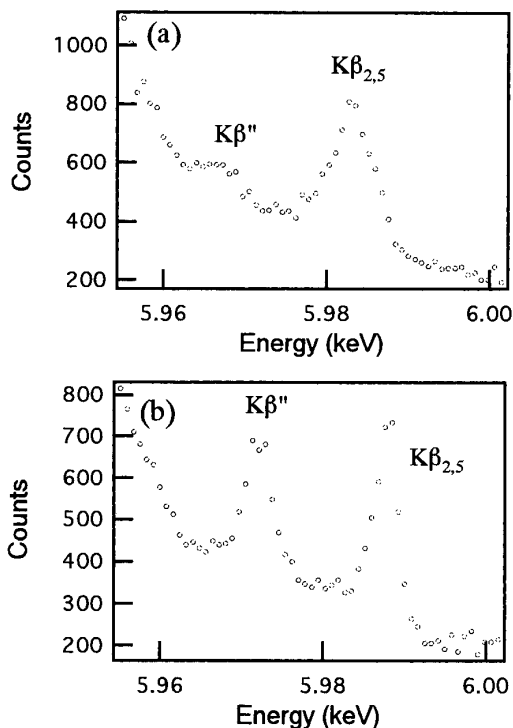


Figure 2. (a): The $K\beta_{2,5}$ and $K\beta''$ spectra of FeCr_2O_4 (octahedral symmetry), (b): The $K\beta_{2,5}$ and $K\beta''$ spectra of $\text{K}_2\text{Cr}_2\text{O}_7$ (tetrahedral symmetry)

FeCr_2O_4 (octahedral symmetry). This way of appearances of the $K\beta''$ satellite line is opposite to that of the $K\beta$ satellite line. It was reported that the origin of the $K\beta''$ satellite line might be ascribed to the molecular orbital [4]. To investigate these lines more precisely the spectra with high S/N are necessary though it is difficult to get because of the weakness of the $K\beta_{2,5}$ lines and $K\beta''$ satellite line.

Tuning the energy of the incident beam, by which we can control the possibility of occurrence of some special processes, gives us useful informations about the effect of various processes on x-ray emission spectra. Recently the advent of synchrotron radiation facility made this kind of experiment possible. Such experiments will help us to solve many problems of x-ray emission spectra.

References

1. K. Tsutsumi, J. Phys. Soc. Jpn. **14**, 1696 (1959)
2. M. Deutsch, G. Hözer, J. Hätwig, J. Wolf, M. Fritsch and E. Förster, Phys. Rev. A, **51**, 283 (1995)
3. K. S. Srivastava *et al.*, Phys. Rev. A, **19**, 4336 (1979); **25**, 2838 (1982)
4. T. Mukoyama, K. Taniguchi, H. Adachi, Phys. Rev. B, **34**, 3710 (1986)