Cr-Kβ X-ray Emission Spectra in Several Chromium Compounds

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Cr- Kβ 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 Kβ' and Kβ" satellite lines are confirmed in the spectra of the compounds. The origin of Kβ' and Kβ" satellite lines is discussed due to both the number of unpaired electrons and the symmetry of ligands around the chromium atom.

Keywords: Kβ' and Kβ" 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 Kβ' and Kβ" satellite lines) the K x-ray emission spectra of chromium in Cr metal, Cr_2O_3, $CoCr_2O_4$, $FeCr_2O_4$, K_2CrO_4 and $K_2Cr_2O_7$ were measured using a double crystal spectrometer with high resolution.

The Kβ' 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$\rightarrow$1s. As can be seen from Figure1, the relative intensity of the Kβ' satellite line to the K$\beta_{1,3}$ lines for compound with octahedral symmetry is larger than that for compound with tetrahedral symmetry. Tsutsumi suggested that the Kβ' 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

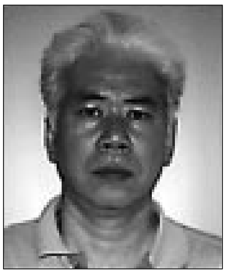
$$\Delta E=J(2S+1),$$

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 Kβ' 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.



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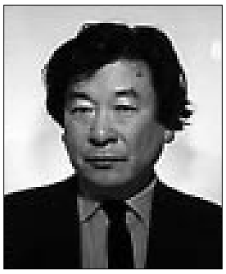

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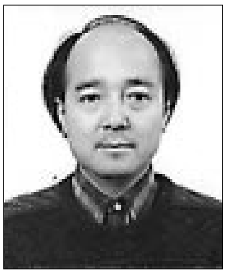

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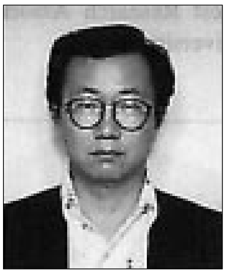

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spectra. According to this theory, the relative intensity of Kβ' satellite lines to the K$\beta_{1,3}$ line is given by S/(S+1). The number of unpaired electrons is formally three (S=3/2) in the compounds with octahedral symmetry, zero (S=0) in the compounds with tetrahedral symmetry. Then this theory can account for the larger intensity of the Kb' lines in the compounds with octahedral symmetry. But it cannot explain the Kβ' satellite line quantatively 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 Kβ' satellite line sufficiently.

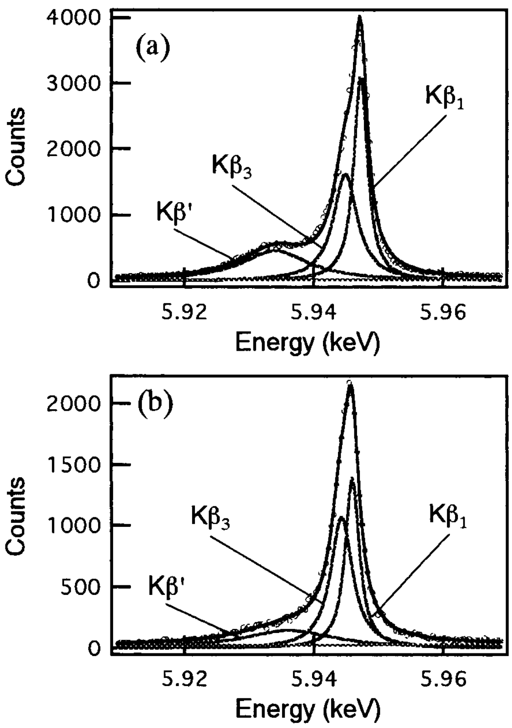

Figure 1. (a): The K$\beta_{1,3}$ and Kβ' spectra of $FeCr_2O_4$ (octahedral symmetry), (b): The K$\beta_{1,3}$ and Kβ' spectra of $K_2Cr_2O_7$ (tetrahedral symmetry)

The Kβ'' satellite lines with the K$\beta_{2,5}$ lines of chromium in $FeCr_2O_4$ (octahedral symmetry) and $K_2Cr_2O_7$ (tetrahedral symmetry) are shown in figure 2. The Kβ'' satellite line appears on the high energy side of the K$\beta_{2,5}$ lines. The Kβ_2 line and the Kβ_5 line are generated by the single electron transition of 4p$\rightarrow$1s and 3d$\rightarrow$1s respectively. It is easily seen that the relative intensity of Kβ'' satellite line to the K$\beta_{2,5}$ lines in $K_2Cr_2O_7$ (tetrahedral symmetry) is much larger than that in

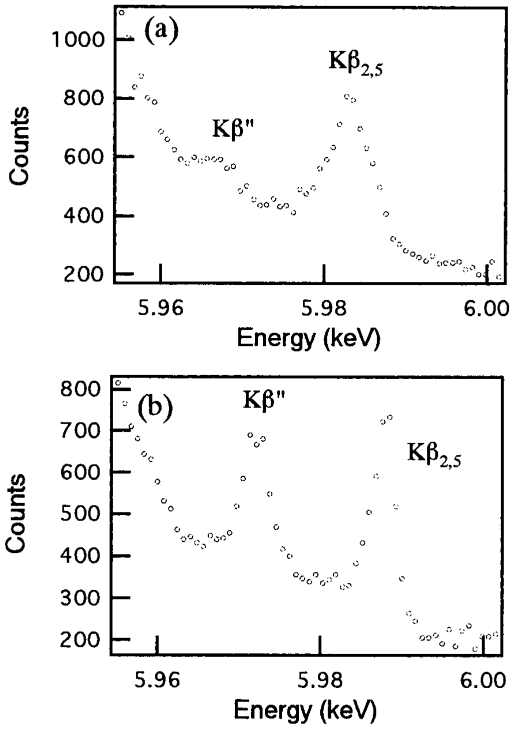

Figure 2. (a): The K$\beta_{2,5}$ and Kβ'' spectra of $FeCr_2O_4$ (octahedral symmetry), (b): The K$\beta_{2,5}$ and Kβ'' spectra of $K_2Cr_2O_7$ (tetrahedral symmetry)

$FeCr_2O_4$ (octahedral symmetry). This way of appearances of the Kβ'' satellite line is opposite to that of the Kβ' satellite line. It was reported that the origin of the Kβ'' 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 Kβ'' satellite line.

Tuning the energy of the incident beam, by which we can controll the posssibility of occurrence of some special processes, gives us useful imformations 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.

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