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Influence of changes in the valence electronic configuration on the $K\beta$-to-$K\alpha$ x-ray intensity ratios of the $3d$ transition metals

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Very extensive multiconfiguration Dirac-Fock calculations including the transverse (Breit) interaction and quantum electrodynamics corrections have been carried out for all $3d$ transition metals to explain reliably the dependence of $K\beta$-to-$K\alpha$ x-ray intensity ratios on the changes in configurations of the valence electrons. For all considered atoms the greatest values of the $K\beta$-to-$K\alpha$ intensity ratios are for $3d^{m-2}4s^2$ configuration type, then for $3d^{m-1}4s^1$, and the smallest values are for $3d^m$ type. It has been found that for each type of electronic configuration the $K\beta$-to-$K\alpha$ intensity ratios increase evidently with the atomic number and for a particular atom they are quite sensitive to the changes of the valence electronic configuration. The greatest relative increase of the $K\beta$-to-$K\alpha$ intensity ratios (4%) as a result of transition from electronic configuration of the $3d^{m-1}4s^1$ type to the $3d^{m-2}4s^2$ type takes place for Sc and the smallest relative increase (2%) takes place for Cu. The presented results make it possible to carry out reliable interpretation of various experimental $K\beta$-to-$K\alpha$ x-ray intensity ratios for $3d$ transition metals in their compounds and alloys and can also provide quantitative information about the changes of the valence electronic configurations of these metals in considered systems. [S1050-2947(98)04708-8]

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I. INTRODUCTION

A great deal of work has been performed on experimental and theoretical studies of the $K\beta$-to-$K\alpha$ intensity ratios in the x-ray spectra. The relativistic equivalent of the one-electron approximation has been used by several authors for theoretical predictions on the $K\beta$-to-$K\alpha$ intensity ratios. Following Scofield [1] the recent studies in this field are based on the use of Dirac-Fock (DF) one-electron wave functions. However, systematic discrepancies between experimental and theoretical results have been found by several authors [2–4]. For the last 11 years Perujo *et al.* [5] have performed high-precision studies of the $K\beta$-to-$K\alpha$ intensity ratios in proton-induced x-ray spectra in the $22 \leqslant Z \leqslant 32$ region and confirmed the systematic discrepancy consisting in overestimating the experimental results by the theoretical predictions of Scofield [1].

In recent years, I have started to develop and apply theoretical models, based on the results of multiconfiguration Dirac-Fock (MCDF) calculations, for reliable descriptions of very complex x-ray spectra of multiply ionized atoms. In a series of papers systematic studies on the structure of various types of $K\alpha$ and $K\beta$ satellite lines in the x-ray spectra of different atoms have been presented [6–10]. The results of these papers have been successfully implemented in analyses of $K\alpha$ and $K\beta$ x-ray spectra of many target atoms (with $Z > 40$) generated in near-central collisions with various light and heavy projectiles [11–16]. In particular, we have investigated the $K\beta$-to-$K\alpha$ x-ray intensity ratios of the $3d$ transition metals [17–19]. In one of the 1989 papers [17], an alternative special average level (SAL) version of MCDF calculations was proposed. It gives values of the $K\beta$-to-$K\alpha$ intensity ratios for Ti, Cr, Fe, Ni, Cu, Zn, and Ge in a significantly better agreement with highly accurate experimental data of Perujo *et al.* [5] than the theoretical predictions of Scofield [1] and the results of standard average level (AL) and extended average level (EAL) versions of MCDF calculations (see Grant *et al.* [20]).

So far most of the experimental studies of the $K\beta$-to-$K\alpha$ intensity ratios have not paid much attention to the influence of chemical environment and solid-state effects. However, some studies made on $3d$ transition-metal compounds [21–29] and alloys [30,31] have shown dependence of the $K\beta$-to-$K\alpha$ ratio on chemical environment or alloy composition. Recently, Padhi and Dhal [32] have measured $K\beta$-to-$K\alpha$ x-ray intensity ratios of Fe, Co, Ni, Cu, Mo, Ru, Rh, and Pd transition metals in equiatomic aluminides following excitation by γ rays and have found the effect of alloying on the $K\beta$-to-$K\alpha$ ratios of the transition metals. In the case of $3d$ transition-metal aluminides they have found significant decrease in the $K\beta$-to-$K\alpha$ ratio with respect to the pure metal value. It has been suggested by Bhuinya and Padhi [30,31] that, although the results on $K\beta$-to-$K\alpha$ x-ray intensity ratios of $3d$ transition metals in various alloys can be qualitatively explained by taking into account the available simple charge-transfer or rearrangement models, systematic calculations based on different electronic configurations of these atoms would be more useful in interpreting the data.

Very recently we have proposed a method for the analysis and interpretation of the measured $K\beta$-to-$K\alpha$ intensity ratios for the $3d$ transition-metal alloys [19], which does indeed fulfill the requirement formulated by Bhuinya and Padhi [30,31]. This method, based on the results of MCDF calculations for different valence electronic configurations of $3d$ transition-metal atoms, not only makes it possible to carry out reliable interpretation of the experimental $K\beta$-to-$K\alpha$ intensity ratios but also provides quantitative information about the changes of the valence electronic configurations of these metals in their compounds and alloys. To the best of my knowledge, no systematic study has been carried out to

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explain the dependence of $K\beta$-to-$K\alpha$ intensity ratios for $3d$ transition metals on the changes in configurations of their valence electrons. Therefore in this paper the results of systematic MCDF calculations in the most accurate (as mentioned above) SAL version have been presented for all $3d$ transition metals considering three valence electronic configurations each belonging to a different one of the three $3d^{m-r}4s^{r}$ ($r=2,1,0$) types. Some results presented in this paper have already been successfully applied to explain reliably the observed $K\beta$-to-$K\alpha$ intensity ratios for Ni and Cu in various silicide compounds [18]. The results of studies presented in this paper have potential applications in the interpretation of various experimental $K\beta$-to-$K\alpha$ intensity ratios for $3d$ transition metals in compounds and alloys.

II. METHODOLOGICAL REMARKS

The MCDF method applied in the present study has been mainly developed by Grant and co-workers and is described in detail in several papers [20,33–38]. Moreover, all basic ideas of the alternative SAL version of MCDF calculations, which is used in this work, have been presented by Jankowski and Polasik [17]. However, for the sake of clarity, some essential details are very briefly recapitulated below.

The Hamiltonian for the N-electron atom is taken in the form (atomic units are used)

$$H=\sum_{i=1}^{N} h_D(i)+\sum_{j>i=1}^{N} C_{ij}, \tag{1}$$

where $h_D(i)$ is the Dirac operator for the ith electron and the terms C_{ij} account for electron-electron interactions and come from one-photon exchange process. The latter are a sum of the Coulomb interaction operator and the transverse Breit operator (due to transversely polarized photons).

The atomic state function with the total angular momentum J and parity p is expanded in terms of configuration state functions (CSF's) as

$$\Psi_s(J^p)=\sum_m c_m(s)\phi(\gamma_m J^p). \tag{2}$$

The CSF's are the antisymmetrized N-electron wave functions built from one-electron spinors, $c_m(s)$ are the configuration mixing coefficients for the state s, and γ_m represents all information required to uniquely define a certain CSF.

In the SAL version of MCDF calculations the energy functional is specially averaged over all the initial and final states and can be expressed by

$$E=E_{\mathrm{opt}}+\sum_a \overline{q_a}\epsilon_a S(a,a)+\sum_{\substack{a,b\\ a\neq b}} \epsilon_{a,b} S(a,b), \tag{3}$$

where $\overline{q_a}$ is the generalized occupation number for the orbital a, ϵ_a and ϵ_{ab} are the Lagrange multipliers, $S(a,b)$ is the overlap integral, and E_{opt} is taken in the form

$$E_{\mathrm{opt}}=\frac{1}{3}\left[\frac{1}{n_i}\sum_{i=1}^{n_i} H_{ii}+\frac{1}{n_j}\sum_{j=1}^{n_J} H_{jj}+\frac{1}{n_k}\sum_{k=1}^{n_k} H_{kk}\right], \tag{4}$$

where H_{ii}, H_{jj}, and H_{kk} are the diagonal contributions to the Hamiltonian matrix, n_i is the number of all the CSF's defining the initial states (of the type $1s^{-1}$), and n_j and n_k are the numbers of all the CSF's defining the final states of the types $2p^{-1}$ and $3p^{-1}$, respectively.

In this version of calculation the common set of the orbitals for all the initial and final states is to be determined. This removes the problem of nonorthogonality of the orbitals and, moreover, greatly reduces the computational effort, as only the coefficients $c_m(s)$ have to be determined for each state by diagonalizing the matrix of the Hamiltonian in the space of relevant CSF's. It is evident that for each particular state such orbitals yield higher energy (the effect of relaxation) than those obtained from the optimal level version (see Grant *et al.* [20]) of MCDF calculations for each state. However, usually all energy levels are shifted by approximately the same extent (see Jankowski and Polasik [17]). The orbitals determined in the SAL version are better suited for calculations of the transition probabilities than those determined in the standard AL version. This is due to the fact that unlike the AL version, where all states are uniformly represented in the energy functional, in the SAL version the weights of the contributions corresponding to the more numerous configurations are reduced in the energy functional. This is a remedy against exaggerating the contribution of the more numerous configurations to the energy functional.

Apart from the transverse (Breit) interaction two types of quantum electrodynamics (QED) corrections are included, namely, the self-energy and vacuum polarization corrections (see McKenzie *et al.* [33]). The formulas for the transition matrix elements and spontaneous emission probabilities can be found in the work of Grant [34]. The calculations have been performed for both the Coulomb and Babushkin [39,40] gauges. In the nonrelativistic limit the Coulomb gauge formula for the electric dipole transitions yields the dipole velocity expression while the Babushkin formula gives the dipole length expression [34]. The studies presented in this paper have been done using the atomic MCDF package developed by Grant and co-workers [20,33].

III. RESULTS AND DISCUSSION

As has been mentioned in the Introduction, the approach to study $K\beta$-to-$K\alpha$ x-ray intensity ratios based on the SAL version of the MCDF method has proved its power and reliability in the case of several $3d$ transition metals [17]. In particular, for the Ni atom the three different valence electronic configurations ($3d^8 4s^2$, $3d^9 4s^1$, and $3d^{10}$) have been considered by Jankowski and Polasik [17]. Therefore I have found it reasonable to apply the SAL version of the MCDF method to study the dependence of $K\beta$-to-$K\alpha$ x-ray intensity ratios on changes in configurations of the valence electrons in the case of all $3d$ transition metals. In this paper the results of systematic studies obtained by performing very extensive MCDF calculations in the SAL version with the inclusion of the transverse (Breit) interaction and QED (self-energy and vacuum polarization) corrections have been presented.

The present calculations differ in several points from the well-known and fundamental work of Scofield [1]. First of all, Scofield does not at all consider transitions between in-

TABLE I. Number of CSF's, number of transitions, and the calculated $K\beta$-to-$K\alpha$ x-ray intensity ratios of $3d$ transition metals corresponding to various valence electronic configurations of the $3d^{m-r}4s^r$ ($r=2,1,0$) types.

					The $K\beta$-to-$K\alpha$ intensity ratios	
Element	Z	Electronic configuration	The total number of CSF's	The number of transitions	Coulomb gauge	Babushkin gauge
Sc	21	$3d^14s^2$	28	72	0.1290	0.1319
		$3d^24s^1$	212	3012	0.1239	0.1272
		$3d^3$	258	4164	0.1204	0.1236
Ti	22	$3d^24s^2$	106	802	0.1308	0.1334
		$3d^34s^1$	500	15822	0.1262	0.1291
		$3d^4$	423	10848	0.1230	0.1259
V	23	$3d^34s^2$	258	4164	0.1322	0.1345
		$3d^44s^1$	846	41424	0.1280	0.1306
		$3d^5$	502	14852	0.1251	0.1276
Cr	24	$3d^44s^2$	423	10848	0.1333	0.1354
		$3d^54s^1$	978	56798	0.1295	0.1317
		$3d^6$	423	10848	0.1268	0.1289
Mn	25	$3d^54s^2$	502	14852	0.1342	0.1361
		$3d^64s^1$	846	41424	0.1307	0.1326
		$3d^7$	258	4164	0.1282	0.1301
Fe	26	$3d^64s^2$	423	10848	0.1349	0.1366
		$3d^74s^1$	500	15822	0.1317	0.1334
		$3d^8$	106	802	0.1294	0.1310
Co	27	$3d^74s^2$	258	4164	0.1356	0.1370
		$3d^84s^1$	212	3012	0.1326	0.1340
		$3d^9$	28	72	0.1304	0.1318
Ni	28	$3d^84s^2$	106	802	0.1361	0.1374
		$3d^94s^1$	54	262	0.1333	0.1346
		$3d^{10}$	5	4	0.1313	0.1325
Cu	29	$3d^94s^2$	28	72	0.1366	0.1377
		$3d^{10}4s^1$	10	12	0.1340	0.1350

dividual states corresponding to the electronic configurations. Instead he represents the whole configuration by a single determinant from single-particle functions obtained from DF equations depending on properly chosen occupation numbers. As a result he obtains different nonorthogonal sets of single-particle functions for the initial and final configurations. The required transition probabilities are expressed in terms of these functions. Moreover, Scofield does not take into account the Breit and QED corrections.

The total number of CSF's, number of transitions, and the calculated $K\beta$-to-$K\alpha$ x-ray intensity ratios of all $3d$ transition metals for three valence electronic configurations each belonging to a different of the three $3d^{m-r}4s^r$ ($r=2,1,0$) types are presented in Table I (preliminary results for the Ni atom have been presented by Jankowski and Polasik [17]). In each case the Coulomb and Babushkin gauge formulas for the electric dipole transitions have been used. From Table I it can be seen that the case of the $3d^{10}$ configuration for the Ni atom is the simplest case as far as the $3d$ transition-metal atoms are concerned, which is caused by the closed-shell nature of the $3d^{10}$ state of the valence electronic configuration of the neutral Ni atom. If for this closed-shell case only one electron from the $1s$ subshell has been removed, just five CSF's are possible (only one CSF for the initial states of the type $1s^{-1}$, two CSF's for the final states of the type $2p^{-1}$, and two CSF's for the final states of the type $3p^{-1}$). For this case we have to consider only four transitions ($K\alpha_1$, $K\alpha_2$, $K\beta_1$, and $K\beta_3$). In the remaining cases the considered atoms are in open-shell states and if one removes one $1s$ electron from such an atom the initial states of the created ion correspond to the configuration which has more than one open subshell. Therefore many CSF's differing in their total angular momentum J are possible for a certain configuration and, moreover, there are usually many different CSF's for a certain J. All this implies transitions between large numbers of initial and final CSF's. Generally, in the presented cases the number of CSF's and the number of transitions depend very strongly on the number of $3d$ electrons (and also on the number of $4s$ electrons) in the $3d^{m-r}4s^r$ ($r=2,1,0$) configurations of the considered atoms. Mostly, the number of CSF's and the number of transitions are very large. In some cases (V for $3d^44s^1$, Cr for $3d^54s^1$, and Mn for $3d^64s^1$) more than 800 CSF's and more than 40 000 transitions can be observed. The most complicated case is for a Cr atom in the $3d^54s^1$ configuration, in which occupation of the $3d$ shell (and moreover the $4s$ shell) is half and half. For this case we have 978 CSF's (144 CSF's for the initial states of the type $1s^{-1}$, 417 CSF's for the final states of the type

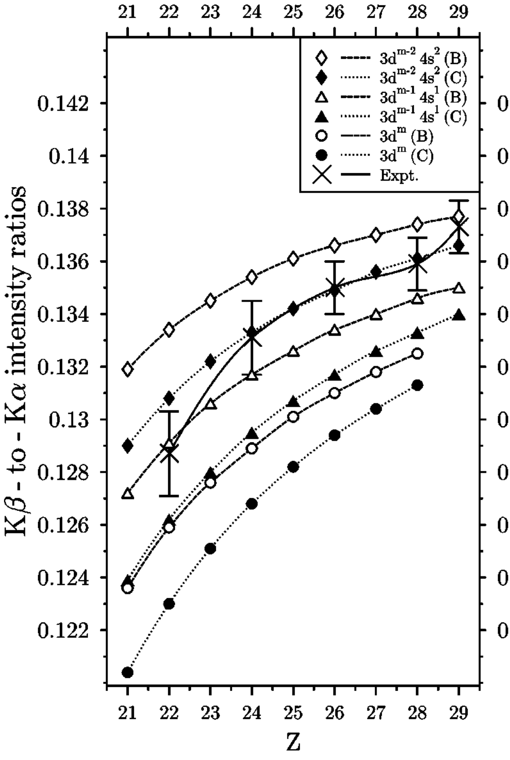

FIG. 1. Comparison of the results of MCDF calculations on the $K\beta$-to-$K\alpha$ x-ray intensity ratios corresponding to all three different valence electronic configurations of all $3d$ transition metals [each belonging to a different one of the three $3d^{m-r}4s^r$ ($r=2,1,0$) types] with the highly accurate experimental $K\beta$-to-$K\alpha$ x-ray intensity ratios (by Perujo *et al.* [5]); "(B)" denotes Babushkin gauge results; "(C)" denotes Coulomb gauge results.

$2p^{-1}$, and 417 CSF's for the final states of the type $3p^{-1}$) and 56 798 transitions.

For better comparison, the results of MCDF calculations of the $K\beta$-to-$K\alpha$ x-ray intensity ratios for all three valence electronic configurations each belonging to a different one of the three $3d^{m-r}4s^r$ ($r=2,1,0$) types are shown in Fig. 1 as functions of the atomic number (Z). For all cases the $K\beta$-to-$K\alpha$ intensity ratios (see Table I and Fig. 1) are always higher for the Babushkin gauge than for the Coulomb gauge. From the data presented in Table I and from Fig. 1 it can be seen that for all three types of valence electronic configurations [i.e., for all the $3d^{m-r}4s^r$ ($r=2,1,0$) types] the $K\beta$-to-$K\alpha$ intensity ratios increase evidently with Z and for a particular atom they are quite sensitive to the changes of the valence electronic configuration. For all atoms the greatest values of the $K\beta$-to-$K\alpha$ x-ray intensity ratios are for $3d^{m-2}4s^2$ configuration type, then for $3d^{m-1}4s^1$, and the smallest values are for $3d^m$ type.

Moreover, in Fig. 1 the results of MCDF calculations are compared with the highly accurate experimental $K\beta$-to-$K\alpha$ x-ray intensity ratios (by Perujo *et al.* [5]). It can be found from Fig. 1 that for Cr, Fe, and Ni the perfect agreement with the experimental results is found for the MCDF results corresponding to the configurations of $3d^{m-2}4s^2$ type and based on the Coulomb gauge, whereas for Cu the results corresponding to the $3d^9 4s^2$ configuration (i.e., $3d^{m-2}4s^2$ type) and based on the Babushkin gauge yield slightly better agreement. Only for Ti is the result corresponding to the $3d^2 4s^2$ configuration (i.e., $3d^{m-2}4s^2$ type) and based on the Coulomb gauge very slightly outside the uncertainty region indicated by Perujo *et al.* [5]. For the Ti atom the best agreement with the experimental results is found for the MCDF results based on the Babushkin gauge and corresponding to the $3d^3 4s^1$ configuration (i.e., $3d^{m-1}4s^1$ type).

The calculated relative increases of the $K\beta$-to-$K\alpha$ intensity ratios as a result of transition from electronic configuration of the $3d^{m-1}4s^1$ type to the $3d^{m-2}4s^2$ type and, for comparison, the relative increases of the $K\beta$-to-$K\alpha$ intensity ratios per one removed $3d$ electron estimated using a very simple semiempirical formula by Brunner *et al.* [24] for all the $3d$ transition metals are presented in Table II. The greatest relative increase (about 4%) of the $K\beta$-to-$K\alpha$ intensity ratios (see the calculated relative increases in Table II) takes place for the Sc atom (the smallest Z value) and the smallest relative increase (about 2%) takes place for the Cu atom (the greatest Z value). It can be noticed that, although the absolute values of the $K\beta$-to-$K\alpha$ intensity ratios obtained using the Coulomb and Babushkin gauges are quite different (see Table I and Fig. 1), the relative changes of the $K\beta$-to-$K\alpha$

TABLE II. Relative effect of changes in the electronic configuration on the $K\beta$-to-$K\alpha$ x-ray intensity ratios of the $3d$ transition-metal atoms. For comparison in the last column the relative increase of the $K\beta$-to-$K\alpha$ intensity ratios per one removed $3d$ electron (after Brunner *et al.* [24]) is also presented.

Element	Changes in the valence electronic configuration	Calculated relative increase of the $K\beta$-to-$K\alpha$ intensity ratios		Relative increase of the $K\beta$-to-$K\alpha$ ratios per one removed $3d$ electron [24]
		Coulomb gauge	Babushkin gauge	
Sc	$3d^2 4s^1 \rightarrow 3d^1 4s^2$	1.041	1.037	
Ti	$3d^3 4s^1 \rightarrow 3d^2 4s^2$	1.036	1.033	1.044
V	$3d^4 4s^1 \rightarrow 3d^3 4s^2$	1.032	1.030	1.040
Cr	$3d^5 4s^1 \rightarrow 3d^4 4s^2$	1.029	1.028	1.030
Mn	$3d^6 4s^1 \rightarrow 3d^5 4s^2$	1.027	1.026	1.035
Fe	$3d^7 4s^1 \rightarrow 3d^6 4s^2$	1.025	1.024	1.030
Co	$3d^8 4s^1 \rightarrow 3d^7 4s^2$	1.023	1.023	1.025
Ni	$3d^9 4s^1 \rightarrow 3d^8 4s^2$	1.021	1.021	1.025
Cu	$3d^{10} 4s^1 \rightarrow 3d^9 4s^2$	1.019	1.020	1.017

intensity ratios as a result of transition from electronic configuration of the $3d^{m-1}4s^1$ type to the $3d^{m-2}4s^2$ type are almost the same (see Table II). These relative increases of the $K\beta$-to-$K\alpha$ intensity ratios are generally in good agreement with semiempirical values by Brunner *et al.* [24] although the MCDF results presented in this paper are for all atoms but Cu slightly lower.

IV. CONCLUSIONS

To explain reliably the dependence of $K\beta$-to-$K\alpha$ x-ray intensity ratios on changes in configurations of the valence electrons for all $3d$ transition metals, very extensive MCDF calculations in the SAL version including the transverse (Breit) interaction and QED corrections have been performed for all three valence electronic configurations each belonging to a different one of the three $3d^{m-r}4s^r$ ($r=2,1,0$) types. On the basis of these calculations some general conclusions can be drawn.

First, the number of CSF's and the number of transitions depend very strongly on the number of $3d$ electrons (and also on the number of $4s$ electrons) in the $3d^{m-r}4s^r$ ($r=2,1,0$) configurations of the considered atoms. In most cases the number of CSF's and the number of transitions are very large. In the most complicated case (Cr for $3d^5 4s^1$ configuration) we have 978 CSF's and 56 798 transitions. Second, for each type of valence electronic configuration the $K\beta$-to-$K\alpha$ intensity ratios increase evidently with the atomic number Z and for a particular atom they are quite sensitive to the changes in configurations of the valence electrons. Third, for all atoms the greatest values of the $K\beta$-to-$K\alpha$ intensity ratios are for $3d^{m-2}4s^2$ configuration type, then for $3d^{m-1}4s^1$, and the smallest values are for $3d^m$ type. Fourth, for all but the Ti atom the $K\beta$-to-$K\alpha$ x-ray intensity ratios calculated for $3d^{m-2}4s^2$ configuration type are in very good agreement with the highly accurate experimental data of Perujo *et al.* [5]. Fifth, the greatest relative effect of changes in the electronic configuration (from the $3d^{m-1}4s^1$ type to the $3d^{m-2}4s^2$ type) on the $K\beta$-to-$K\alpha$ intensity ratios (increase about 4%) takes place for Sc (the smallest Z value) and the smallest relative effect (increase about 2%) takes place for Cu (the greatest Z value). These relative increases of the $K\beta$-to-$K\alpha$ intensity ratios are generally in good agreement with semiempirical values by Brunner *et al.* [24].

The author believes that the results of this work will be helpful in better understanding of the dependence of $K\beta$-to-$K\alpha$ x-ray intensity ratios on changes in the valence electronic configurations of $3d$ transition metals and can be used to find proper theoretical explanation of the influence of chemical environment and solid-state effects on the $K\beta$-to-$K\alpha$ intensity ratios of these metals in various compounds and alloys. They also provide a sensitive tool to study quantitatively the changes of the valence electronic configurations of $3d$ transition metals in such systems.

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