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Spectra and oscillator strengths of $3p^63d^9$–$3p^53d^{10}$ and $3p^63d^9$–$3p^63d^84p$ transitions for cobalt-like Sn^{23+} ion*

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This paper calculates the spectra and oscillator strengths for highly ionized cobalt-like Sn^{23+} ions $3p^63d^9-3p^53d^{10}$, $3p^63d^9-3p^63d^84p$ transitions by using a multi-configuration self-consistent field method program together with the proposed fitting formula. The calculations have a good agreement with observations.

Keywords: highly ionized, energy level, the fitting formula
PACC: 3270, 3270C, 3270F

1. Introduction

The proposition of soft-x-ray laser theory, for which the laser work material is cobalt-like Au^{52+} was verified by T1AP crystal spectrograph.[1] That renewed the research interest in highly ionized cobalt-like ions. Ions of the cobalt isoelectronic sequence have the ground configuration $3p^63d^9$. At the beginning of the sequence the lowest configuration with odd parity is $3p^63d^84p$. However, from Rb^{10+} on, the $3p^53d^{10}$ configuration takes its place. The correction between $3p^63d^9/^2D$ and $3p^53d^{10}/^2P$ gives rise to configuration combination.

Experimentally, these configuration transitions of cobalt-like ions were first observed by Edlén for Rb, Sr, Y, Zr, Mo, Pd, Ag, Cd, In, and Sn, although no wavelengths were reported.[2] Edlén's observed wavelengths can be inferred from the wave numbers given in his monograph, which also gives values for Br and Sb.[3] Later, Alexander reported wavelengths for these transitions in Y, Zr, Nb, and Mo.[4] Two of these transitions were observed by Burkhalter *et al* for Sn^{23+} in a laser-produced plasma.[5] Burkhalter *et al*[6] reported new wavelength values for Mo^{15+}. The same transitions in Sr^{11+} were given by Acquista and Reader[7] and revised values for Sr^{11+}, Y^{12+}, Zr^{13+}, Nb^{14+}, and Mo^{15+} by Ryabtsev and Reader.[8] The $3p^63d^9-3p^53d^{10}$ transitions of Ba^{29+}, La^{30+}, Nd^{33+}, Sm^{35+}, Gd^{37+}, Dy^{39+}, Er^{41+}, and Yb^{43+} were reported by Reader.[9] New wavelengths for these transitions in Ag^{20+}, Cd^{21+}, In^{22+}, and Sn^{23+} were given by Kononov *et al*.[10] The magnetic-dipole transition between the levels of the $3p^63d^9/^2D$ ground term has been observed in three cobalt-like ions: the magnetic-dipole transitions of Zr^{13+} and Mo^{15+} were observed in the plasmas of laser thermonuclear tokamak by Suckewer *et al*;[11] that of Nb^{14+} was observed in an electron cyclotron resonance ion source by Prior.[12] Ekberg *et al*[13] gave new measurements for $3p^63d^9-3p^53d^{10}$ transitions of the ions from Sr^{11+} to Au^{52+} in laser-produced plasmas.

This paper has theoretically calculated the wavelengths and oscillator strengths for highly ionized cobalt-like Sn^{23+} ions $3p^63d^9-3p^53d^{10}$, $3p^63d^9-3p^63d^84p$ transitions using multi-configuration self-consistent field method[14] together with the fitting formula proposed by us. The calculations have a good agreement with observations.

2. Fitting formulas

Up to the present day, it is difficult to solve a Hartree–Fock–Roser (HFR) equation of polyelectron system accurately. However, our real purpose is calculating accurately the known energy levels of atoms and predicting the unknown energy levels, which can be achieved by using multi-configuration self-consistent field method together with fitting formula. So it is important to find a better fitting formula. Be-

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cause the difference values ΔE between experimental measuring values and theoretical calculated values of multi-configuration self-consistent field method change smoothly along the isoelectronic sequence, we can achieve the least square fitting and find the fitting formula between ΔE and $Z_{\rm c}$. In 1987, Wyart proposed a fitting formula:[15]

$$E_{\rm fit} = -98751.4 + 55078 \times Z_{\rm c} + 5618.86 \times Z_{\rm c}^2 + 7.6414 \times Z_{\rm c}^3 + 7145 \times Z_{\rm c}^4. \quad (1)$$

In 1991, Matsushima proposed another fitting formula:[16]

$$E_{\rm fit} = A + BZ_{\rm c} + CZ_{\rm c}^2/10 + DZ_{\rm c}^3/100 + EZ_{\rm c}^4/1000 + FZ_{\rm c}^5/1000000. \quad (2)$$

According to the quantum electrodynamics effect of high-Z ions proposed by Harvey *et al*,[17] which can move the energy levels of the isoelectronic sequence, we find that the quantum electrodynamics effect of high-Z ions is not considered in Eqs.(1) and (2). So we have proposed a better formula, in which the quantum electrodynamics effect of high-Z ions is included, and it is expressed as

$$\Delta E = A + BZ_{\rm c} + CZ_{\rm c}^2 + DZ_{\rm c}^3 + EZ_{\rm c}^4 + FZ_{\rm c}^5 + GZ_{\rm c}^6 + HZ_{\rm c}^7 + \text{Higher order terms}, \quad (3)$$

where A, B, C, D, E, F, G, H are undetermined parameters; $Z_{\rm c}$, $Z_{\rm c}^2$, $Z_{\rm c}^3$, $Z_{\rm c}^4$ and constant term are used for eliminating high order relativistic effect, remnant correlation energy and radiative corrections; $Z_{\rm c}^5$ is used for eliminating high order Breit effect as in Eqs.(1) and (2). $Z_{\rm c}^6$, $Z_{\rm c}^7$, and higher order terms are used for eliminating the quantum electrodynamics effect of high-Z ions, which is proposed by us. All of above-mentioned effects are not considered by the multi-configuration self-consistent field method program (Cowan's HFR program pack). In this paper, all of these effects are added in calculation results through the fitting formula (3).

The reasonableness of the fitting formula (3) is expressed as follows. Because the electric field of atomic nucleus is stronger than that of atomic electrons for highly ionized ions, the electronic orbit of highly ionized ions is similar to that of hydrogen-like ions. For the hydrogen-like ions, its radial wavefunction can be expressed as

$$P_{nl}(r) = -\left[\frac{Z(n-1-1)!}{n^2[(n+1)!]^3}\right]^{1/2} \times \rho^{l+1}{\rm e}^{-\rho/2} L_{n+1}^{2l+1}(\rho), \quad (4)$$

$$L_{n+1}^{2l+1}(\rho) = [(n+1)!] \times \sum_{k=1}^{2n-l-1} \frac{(-\rho)^k}{(n-l-1-k)! \times (2l+1+k)}. \quad (5)$$

The energy between electrons and atomic nucleus is

$$E_{l-n}^{nl} = \left\langle nl \left| \frac{2Z}{r} \right| nl \right\rangle \propto Z^2. \quad (6)$$

The kinetic energy of electrons is

$$E_{\rm kin}^{nl} = \langle nl | -\nabla^2 | nl \rangle = \left\langle nl \left| -\frac{{\rm d}^2}{{\rm d}r^2} + \frac{l_i(l_i+1)}{r^2} \right| nl \right\rangle \propto Z^2. \quad (7)$$

The Coulomb energy between electrons and electrons is

$$E_{\rm C-C}^{nl,n'l'} = \left\langle nl, n'l' \left| \frac{2}{r_{1,2}} \right| nl, n'l' \right\rangle - \left\langle nl, n't' \left| \frac{2}{r_{1,2}} \right| n'l', nl \right\rangle \propto Z. \quad (8)$$

Considering the relativistic effect, we find that the energy change is

$$E_{\rm m}^{nl} = \frac{a^2}{2} \int_0^\infty P_{nl}(r)[\varepsilon_i - V(r)^i]^2 \times P_{nl}(r){\rm d}r \propto Z^5. \quad (9)$$

Considering radiative corrections, the energy change is

$$E_{\rm kin}^{nl} \propto (Z - S_1)^2, \quad E_{\rm e-N}^{nl} \propto Z(Z - S_2)^3, \quad (10)$$

$$E_{\rm e-e}^{nl,n'l'} \propto (Z - S_3), \quad E_{\rm M.D} \propto (Z - S_4)^4. \quad (11)$$

Finally, considering the quantum electrodynamics effect of high-Z ions,[17] we find that the energy change is

$$E_{\rm QED} = n^{-3}(2\pi)m_0c^2\{[A_{40} + A_{41}\ln](Za)^{-2}\}(Za)^4 + A_{50}(Za)^5 + \{[A_{60} + A_{61}\ln](Za)^{-2} + A_{62}\ln^2(Za)^{-2}\}(Za)^6 + A_{70}(Za)^7 + \text{higher order terms} \propto Z^4, Z^5, Z^6, Z^7 \ldots. \quad (12)$$

In the fitting formulae (1) and (2), the $Z_{\rm c}$, $Z_{\rm c}^2$, $Z_{\rm c}^3$, $Z_{\rm c}^4$, $Z_{\rm c}^5$ and constant term are included, but the $Z_{\rm c}^6$, $Z_{\rm c}^7$ and higher order terms are not included, in which the quantum electrodynamics effect of high-Z ions is not considered. In our fitting formula (3), the $Z_{\rm c}^6$, $Z_{\rm c}^7$ and higher order terms are included so that the quantum electrodynamics effect of high-Z ions is considered, in which we suppose that the energy changes of all configurations caused by higher order terms are same and it is similar to the processing method of Refs.[15, 16].

3. Calculation procedures

Cowan's HFR program pack is used for our calculation, in which relativistic effect and Breit effect are considered already. According to selection rules of transitions and considering configuration combination, we select even parity configurations as $3p^63d^9$, $3p^63d^84s$, $3p^63d^84d$, $3p^63d^85s$, $3p^53d^94p$, $3p^53d^94f$ and odd parity configurations as $3p^53d^{10}$, $3p^63d^84p$, $3p^63d^84f$, $3p^53d^94s$, $3p^53d^94d$, $3p^53d^95s$. The Slater integral factor is selected as 0.95. Because the high order relativistic effect, the remnant correlation energy, the radiative corrections, the high order Breit effect and the quantum electrodynamics effect of high-Z ions are not considered in Cowan's HFR program pack, we need to revise calculation results of the program using the fitting formula (3) proposed by us.

4. Results and discussions

Using the multi-configuration self-consistent field method together with the fitting formula (3) proposed by us, we have calculated energy levels, transitions and oscillator strength of highly ionized cobalt-like Sn^{23+} ions $3p^63d^9$, $3p^53d^{10}$, $3p^63d^84p$ configurations. The fitting parameters of energy level are shown in Table 1 and the fitting values of energy level are shown in Table 2. From Table 2, the difference values between fitting and experimental values are less than $50\,cm^{-1}$.

Table 1. Fitted parameter values of energy levels determined for cobalt-like Sn^{23+} ions.

JN_{th}	A	B	C	D	E	F	G	H
$3p^63d^9$								
$2D_{5/2}$	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0
$2D_{3/2}$	–2024.91	604.141	–65.5063	2.92561	–0.4444955	0.00331144	–0.000526368	0.0000247112
$3p^53d^{10}$								
$2P_{1/2}$	–74732.66	26434.64	–2506.633	101.6266	–1.649258	0.113669	–0.01608	0.00525402
$2P_{3/2}$	–30246.8	15791.1	–1568.82	65.9696	–1.02663	0.0916599	–0.00671575	0.000224571
$3p^63d^84p$								
$4D_{3/2}$	28262400	–8087120	863323	–40771.4	718.979	–11.5441704	0.3443602	–0.01898167
$4P_{3/2}$	–2437540	694519	–74021.4	3497.43	–61.775	7.1548204	–0.15523201	0.0164119
$2D_{1/2}$	–69407	22603.4	–2769.81	149.716	–2.97499	0.2332896	–0.01101523	0.0257287
$2P_{1/2}$	6144790	–1711260	178648	–8271.72	143.367	–9.5390701	0.23643613	–0.0171815

Table 2. Fitted $3p^63d^9$, $3p^53d^{10}$, $3p^63d^84p$ energy levels of cobalt-like Sn^{23+} ions (Unit $\times 1000\,cm^{-1}$).

JN_{th}	E_{fit}	$E_{fit-exp}$
$3p^63d^9$		
$2D_{5/2}$	0.0	0.0
$2D_{3/2}$	73.0574	0.0095
$3p^53d^{10}$		
$2P_{1/2}$	2197.4651	–0.0128
$2P_{3/2}$	1833.9407	–0.0009
$3p^63d^84p$		
$4D_{3/2}$	3937.5559	0.0121
$4P_{3/2}$	3733.0578	–0.0126
$2D_{1/2}$	5350.1055	0.0004
$2P_{1/2}$	5680.2501	–0.0368

It indicates that our theoretical calculation is successful. According to selection rules of configuration transition $\Delta J = J - J' = 0, \pm 1$ (except $J = J' = 0$), we have calculated the wavelengths of cobalt-like Sn^{23+} ions $3p^63d^9 - 3p^53d^{10}$, $3p^63d^9 - 3p^63d^84p$ transitions, which are shown in Table 3. From Table 3, the difference values between fitting and experimental values are less than 0.005 nm. It indicates that the data in this paper are accurate.

Table 3. Fitted $3p^63d^9 - 3p^53d^{10}$, $3p^63d^9 - 3p^63d^84p$ transitions (unit: nm) and oscillator strengths of cobalt-like Sn^{23+} ions.

$JN_{th} - JN_{th}$	$\lambda_{fit'}$	$\lambda_{fit-exp}$	gf
$3p^63d^9 - 3p^53d^{10}$			
$2D_{5/2} - 2P_{3/2}$	54.536	0.005	0.007
$2D_{3/2} - 2P_{1/2}$	47.297	–0.002	0.348
$2D_{3/2} - 2P_{3/2}$	56.189	–0.003	0.021
$3p^63d^9 - 3p^63d^84p$			
$2D_{5/2} - 4D_{3/2}$	12.890	0.004	0.401
$2D_{5/2} - 4P_{3/2}$	22.056	0.002	0.781
$2D_{3/2} - 4D_{3/2}$	17.981	0.005	0.020
$2D_{3/2} - 4P_{3/2}$	24.945	0.002	0.066
$2D_{3/2} - 2D_{1/2}$	23.425	–0.001	0.031
$2D_{3/2} - 2P_{1/2}$	23.142	–0.003	0.291

In our results, the transitions of cobalt-like Sn^{23+} ions are not within soft-x-ray wavelength (2.33 nm–4.36 nm). It is necessary that we continue to calculate other cobalt-like ions or other isoelectronic sequence ions. At the present time, we do not find the data of MCDF method about the wavelengths of cobalt-like Sn^{23+} ions $3p^63d^9 - 3p^53d^{10}$, $3p^63d^9 - 3p^63d^84p$ transitions. Although we do not find the transitions within soft-x-ray wavelength, our results will benefit the heavy ions reaction and scattering.[18−21]

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