Theoretical Atomic Structure Data for Sn and Xe Ions

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Abstract

Excitation energies, transition rates and oscillator strengths for Sn and Xe ions have been calculated using multireference relativistic configuration interaction method based on the no-pair Dirac-Coulomb-Breit Hamiltonian.

Keywords:

1. Introduction

Sn and Xe ions recently attract a considerable attention to people who are developing extreme ultraviolet (EUV) light sources which can emit a light of 13.5 nm wavelength. This precise wave length for the light source comes from an requirement of the optical system of the lithography machine designed. Recently Nishihara *et. al.* [1] has observed EUV spectra from Sn plasma produced by use of a powerful laser light. The experimental spectra consists of a broad peak spread over a wavelength region around 13.5 nm in which the 4d-4f transitions in Sn ions play a major role for the emission. To analyze the experimental spectra, an appropriate plasma model with accurate atomic data for the structure of ions in the plasma is needed. However, it is not always easy to obtain accurate atomic data such as the transition energy with theoretical relativistic calculation because accuracy for transition energies in each ions up to 6 digits is required to obtain accurate transition energies in ions. Moreover, numerical error in obtaining higher n orbitals and the Breit and QED corrections for total energies becomes large. To obtain reliable atomic data, we have carried out accurate calculations of excitation energies in Sn ions and Xe ones with relativistic configuration-interaction (RCI) atomic code [2,3], where an analytical Gaussian-type function (GTF) basis set is used.

2. The effective many-body Hamiltonian

An effective many-body Hamiltonian most commonly used for relativistic atomic structure calculations is taken to be relativistic "no-pair" Dirac-Coulomb-Breit (DCB) Hamiltonian;

$$H_+^{DCB} = \sum_i h_D(i) + \mathcal{L}_+ \left(\sum_{i>j} V_{ij}^{CB} \right) \mathcal{L}_+ \qquad (1)$$

where (in a.u.) h_D is the one-electron Dirac Hamiltonian

$$h_D(i) = c\alpha_i \cdot \boldsymbol{p}_i + c^2(\beta_i - 1) + V_{nuc}(r_i) \qquad (2)$$

and the effective electron-electron interaction $V_{ij}^C B$ is given by the classical instantaneous Coulomb interactions between electrons and low-frequency Breit interaction:

$$V_{ij}^{CB} = r_{ij}^{-1} + B_{ij} \qquad (3)$$

Here α and β are the 4×4 Dirac vector and scalar matrices, respectively. $V_{nuc}(r_i)$ is the nuclear attraction term and B_{ij} read:

$$B_{12} = -\frac{1}{2r_{12}} \left[\alpha_1 \cdot \alpha_2 + (\alpha_1 \cdot \boldsymbol{r}_{12})(\alpha_2 \cdot \boldsymbol{r}_{12})/r_{12}^2 \right] \quad (4)$$

2.1 Matrix Dirac-Fock SCF method

The relativistic independent electron models derived from the no-pair DC Hamiltonians are the Dirac-Fock-Coulomb Self Consistent Field (DFC SCF) methods. Variation of the energy in terms of the DC Hamiltonians leads to pseudo-eigenvalue equations of the form [4,5]:

$$F_\kappa \phi_{n\kappa} = \varepsilon_{n\kappa} \phi_{n\kappa} \qquad (5)$$

where F is the effective one-electron Hamiltonian for the DFC or Dirac-Fock-Breit (DFB) SCF equation, solved self-consistently. The effective one-electron Hamiltonian for the κ-th symmetry takes the form,

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$$F_\kappa = \begin{pmatrix} V_N + U^{LL} & c\Pi_\kappa + U^{LS} \\ c\Pi_\kappa^+ + U^{SL} & V_N + U^{SS} - 2c^2 \end{pmatrix} \qquad (6)$$

with

$$\Pi_\kappa = -d/dr + \kappa/r \quad and \quad \Pi_\kappa^+ = d/dr + \kappa/r$$

Here

$$\phi_{n\kappa} = \begin{pmatrix} P_{n\kappa}(r) \\ Q_{n\kappa}(r) \end{pmatrix} \qquad (7)$$

where $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are referred to as the large and small component of radial functions, respectively. $V_N(r)$ is the nuclear attraction term. The nucleus is modeled as a sphere of uniform proton charge distribution. U^{AB} (A, $B = L$ or S) is the one-body mean-field potential and accounts approximately for electron-electron interaction in the SCF scheme.

In our matrix DFC SCF calculations, both $P_{n\kappa}(r)$ and $Q_{n\kappa}(r)$ are expanded in terms of a set of Gaussian-type functions, $\{X_{\kappa i}^L\}$ and $\{X_{\kappa i}^S\}$:

$$P_{n\kappa}(r) = \sum_i X_{\kappa i}^L C_{n\kappa i}^L \qquad (8)$$

and

$$Q_{n\kappa}(r) = \sum_i X_{\kappa i}^S C_{n\kappa i}^S \qquad (9)$$

where

$$\begin{aligned} X_{\kappa i}^L &= N_L r^{|\kappa|} exp(-\xi_{\kappa i} r^2) \quad for \;\; \kappa < 0 \\ &= N_L r^{\kappa+1} exp(-\xi_{\kappa i} r^2) \quad for \;\; \kappa > 0 \end{aligned} \qquad (10)$$

and

$$X_{\kappa i}^S = N_S \Pi_\kappa^+ X_{\kappa i}^L \qquad (11)$$

Here the $\{C_{n\kappa i}^L\}$ and $\{C_{n\kappa i}^S\}$ are linear variation parameters. N_L and N_S are the normalization factors.

3. Computational details

Matrix DFC SCF and MR-SD CI calculations of the thin and xenon ions Sn^{+9} to Sn^{+14} and Xe^{+8} to Xe^{+11} were performed by using large even-tempered basis sets of G-spinors. The order of the partial-wave expansion included in the virtual space is $L_{max} = 4$. Even tempered G-spinor basis set of 25s21p18d16f16g with $\alpha = 0.14$ and $\beta = 2.0$ were used. All calculations were done with a finite nucleus of uniform proton charge distribution.

Single-configuration matrix Dirac-Fock SCF calculations (Breit interaction not included) were performed on closed-shell to obtain radial wavefunctions of occupied and virtual orbitals. These orbitals are common in all Atomic State Functions regardless J and parity.

Configuration State Functions (CSF) were constructed by single and double excitations up to $n = 7$ from reference states.

4. Results

In this paper only part of our results is presented. Behavior of Sn^{+12} spectra with respect to the different types of CSF's space is analyzed.

Radial wave functions were obtained by means matrix DFC SCF method. Energy levels of Sn^{+12} were calculated for total angular momentum $J = 0$ to 5 of both parities by means multireference (MR) RCI method. Values of oscillator strength for Sn^{+12} are plotted on Figs. 1, 2 and 3. Spectra plotted on Fig. 1 were obtained by MR RCI calculation for CSF's space constructed by single and double (SD) excitations from several reference states. All core orbitals up $n = 3$ were frozen, only SD excitation from $n = 4$ shells up to $n = 7$. The order of the partial-wave expansion included in the virtual space is $L_{max} = 4$. CSF's space for spectra presented on Figs. 2 and 3 were obtained by SD excitations from the same reference states and same set of radial orbitals as for Fig. 1 spectrum but 3d orbital was open for excitations. Excitations up to $n = 4$ and $n = 5$ were included in CSF's space for spectra displayed on Figs. 2 and 3, respectively. The spectrum on Fig. 1 is significantly shifted to the shorter waves compare to the spectra on Figs. 2 and 3. That shift may be interpreted in the following way: basic configuration of the level composition for the most of excited states consist of 4d orbitals($4d^2$, $4d^3$, 4d4f etc.). 4d orbitals strongly interacts with 3d; including this interaction in CI calculation gives significant changes in energy level position.

In conclusion, despite enormously grow of CSF space, 3d and possibly 3p orbitals should be taken into account in CI calculations.

References

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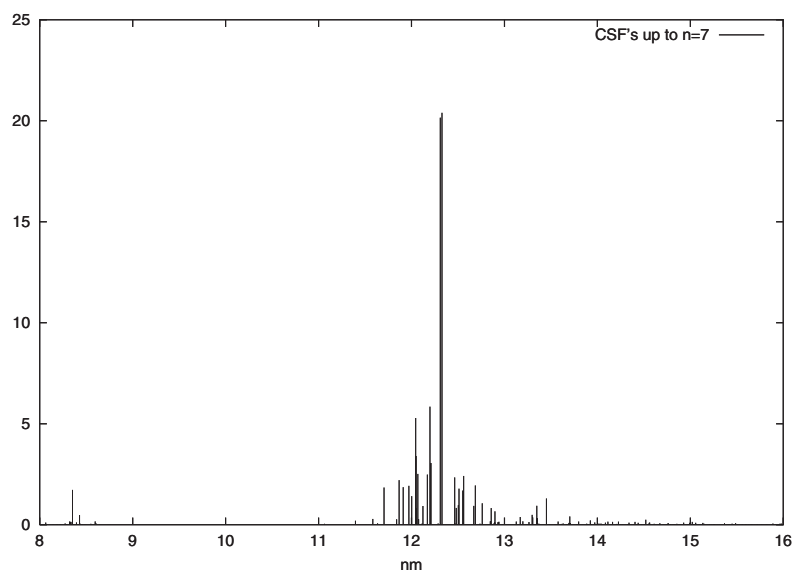[5] Y. Ishikawa, R. Baretty and Jr.R. C. Binning, Chem. Phys. Lett. **121**, 130 (1985).

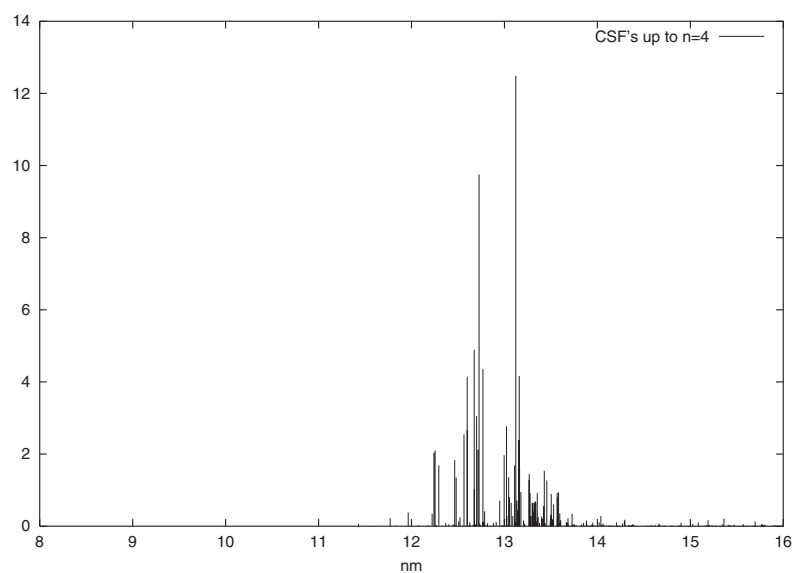Fig. 1   gf values for Sn^{+12} ion: SD excitations from $n=4$ shells

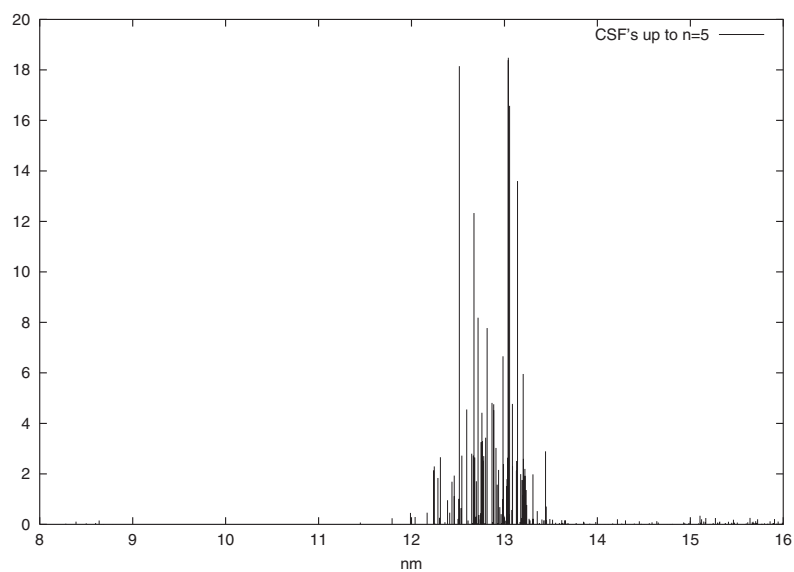Fig. 2   gf values for Sn^{+12} ion: SD excitations from 3d and $n=4$ shells

Fig. 3   gf values for Sn^{+12} ion: SD excitations from 3d and $\boldsymbol{n = 4}$ shells