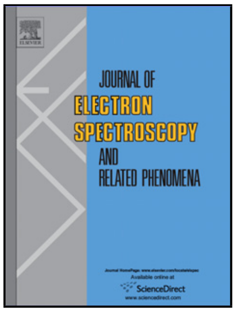

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Electron impact ionization cross sections of the ground and excited levels of Se^{3+}

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Electron impact single ionization cross sections are theoretically investigated from the ionization threshold to 1000 eV for the levels belonging to the ground and two lowest excited configurations of $([Ni])4s^24p$, $4s4p^2$, and $4s^24d$ of Se^{3+} using a detailed level-to-level distorted-wave formalism. The ionization cross sections of the two levels belonging to the configuration of $4s^24p$ are nearly equivalent and so are $4s^24d$, whereas large difference is found for the eight levels of $4s4p^2$. The theoretical results are utilized to analyze and interpret a recent experimental measurement for the single-ionization cross section of Se^{3+} [Alna′washi G A *et al.* 2014 J. Phys. B **47** 135203]. The population distributions existed in this experiment are deduced. Except for the levels of the ground configuration, there exist populations from levels of the excited configuration of $4s^24d$.

I. INTRODUCTION

Electron impact ionization cross section plays an important role in various research fields such as astrophysics [1], inertial confinement fusion and plasma modeling [2]. Accurate ionization cross section is crucial to determine the charge state distribution in collisional ionization equilibrium, power balance, impurity composition and to infer the physical conditions of astrophysical and laboratory plasmas such as electron temperature and electron density [3]. The ongoing efforts to improve the accuracy of calculations in astrophysics can be found in Refs. [1, 3].

Atomic data of electron impact ionization of selenium is important in astrophysics. In a large-scale survey of neutron(n)-capture elements in Galactic planetary nebulae, the emission lines of Se^{3+} 2.287 μm in 81 of 120 observed objects were detected [4, 5]. To determine Se elemental abundance, one needs a large amount of atomic data including electron impact ionization cross sections. Very recently, Alna′washi *et al.* [6, 7] experimentally measured the electron impact ionization cross sections of Se^{2+} and Se^{3+} using the dynamic-crossed-beams technique. They compared their measured ionization cross sections with direct ionization (DI) cross sections predicted by the Lotz semi-empirical formula [8], which is much smaller than their measured value. To identify other possible indirect ionization pathways, they [6, 7] calculated the inner-shell configuration averaged ionization energies using the Cowan Hartree-Fock atomic structure code [9]. By comparing the theoretical ionization energies with their experiment, they suggested that the single ionization cross section is dominated by contributions of the excitation-autoionization (EA) of inner-shell electrons. To the best of our knowledge, only one theoretical work reported electron impact ionization cross section for the ground configuration of Se^{3+} ions [10]. Only considering the ground configuration cannot explain the experiment [7].

In this work, we theoretically investigate the electron impact single ionization cross section of the levels belonging to the ground and two lowest excited configurations of $4s^24p$, $4s4p^2$, and $4s^24d$ of Se^{3+} and try to explain the experiment by Alna′washi *et al.* [7]. In electron-impact ionization experiments, it is well known that considerable population of metastable excited states might be produced [11]. In order to interpret the experiment and diagnose the population distribution, we require cross sections of the ground level as well as the excited states.

II. THEORETICAL METHOD

Theoretical calculations were carried out using the Flexible Atomic Code (FAC) developed by Gu [12]. It utilizes a distorted-wave approximation to describe the electron impact ionization and excitation processes. In our previous work [13–15], we have given theoretical details for investigating electron impact ionization cross sections of atomic ions. In the following we only give an outline of the theoretical method.

The atomic structure is determined by diagonalizing the relativistic Hamiltonian of the atomic system involved through solving the Dirac equation. A bound atomic state is constructed by a linear combination of configuration state functions, which are antisymmetric sums of the products of N one-electron Dirac spinors. The continuum orbitals are obtained by solving the Dirac equation with the same central potential as for the bound ones. Once the wavefunctions of the bound and continuum orbitals are determined, the electron impact excitation (EIE) and ionization cross sections can be obtained. The former reads as

$$\sigma_{if} = \frac{2\pi}{k_i^2 g_i} \sum_{\kappa_i\kappa_f} \sum_{J_T} (2J_T+1)| < \psi_i\kappa_i, J_TM_T| \times \sum_{p<q} \frac{1}{r_{pq}} |\psi_f\kappa_f, J_TM_T > |^2 \qquad (1)$$

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