COMMUNICATIONS IN COMPUTATIONAL PHYSICS
Vol. **2**, No. 4, pp. 795-805

Commun. Comput. Phys.
August 2007

A Numerical Study for Dielectronic Recombination Processes in He-Like Argon

Hong Zhang*, Yueming Li, Jun Yan and Jianguo Wang

The Key Laboratory of Computational Physics, Institute of Applied Physics and Computational Mathematics, Beijing 100088, P. R. China.

Received 3 May 2006; Accepted (in revised version) 16 November 2006
Available online 15 February 2007

Abstract. *Ab initio* calculations of dielectronic recombination (DR) processes from the ground state $1s^2$ of He-like argon ion through doubly excited states $1s2snl$, $1s2pnl$ (n=2 to 9) of Li-like argon ions are performed using the multi-configuration Hatree-Fock method with relativistic correction. The theoretical method and its corresponding computation will be outlined. For higher doubly excited states with $n>9$, the scaling law is used to extrapolate the Auger and radiative transition rates. The total and state-to-state cross sections with corresponding rate coefficients in the temperature from 10^2 eV to 10^6 eV are presented, as well as the DR strengths for all the separate resonances. Moreover, peculiarities of the DR from doubly excited $1s2s3l'$ configurations are analyzed and the contributions of two-electron-one-photo (TEOP) radiative transitions to the DR cross sections are also investigated, such as $1s2s^2 \rightarrow 1s^2 2p$, due to the strong configuration interactions. Our theoretical results appear to be in excellent agreement with the previous and recent experimental measurements.

PACS (2006): 34.80.Lx

Key words: Multi-configuration Hatree-Fock method, dielectronic recombination, TEOP.

1 Introduction

Dielectronic recombination was first proposed by Massey and Bates [1] to explain rapid electron-ion recombination rates in the ionosphere. In this process the radiationless capture of a free electron by a recombining ion, forming a doubly excited state, is followed by radiation emission to form a stable singly excited state in the recombined ion. It is an important recombination mechanism to affect the ionization balance and radiative properties in high-temperature dilute plasmas, such as the solar corona [2,3] and thermonuclear fusion plasmas [4]. In recent years, DR is also found to be very significant in

*Corresponding author. *Email addresses:* zhang_olek@126.com (H. Zhang), li_yueming@iapcm.ac.cn (Y. Li), yan_jun@iapcm.ac.cn (J. Yan), wang_jianguo@iapcm.ac.cn (J. Wang)

high density plasmas, such as for X-ray lasers and Inertial Confinement Fusion. The dielectronic satellites also apply to diagnose plasma densities [5] and electron temperatures [6,7] in the high density plasmas.

Argon is frequently employed in fusion devices, since it can easily be injected into the devices, efficiently pumped out and served as a tracer for diagnosing ion temperature by Doppler broadening measurements [8] and plasma rotation profiles by Doppler shifts of x-ray lines [9]. Especially, the characteristic x-ray emission from He-like Argon has been utilized to diagnose the hot plasmas ranging from the magnetically confined or laser-produced plasmas in laboratory, to plasmas of astrophysical objects, such as supernova remnants or solar flares. The experimental studies of DR processes in He-like ions have been performed for several elements by using EBIT, EBIS, or heavy-ion storage ring devices [10-16]. A recent DR experiment on He-like argon at EBIT by Zou et al. [17] shows that the TEOP transition $1s2s^2 \to 1s^2 2p$ has an anomalous high intensity. Such transition has also been observed in a DR experiment by Rosmej [18]. Because the TEOP transition has high sensitivity to the multi-electron wave functions used in theoretical calculations, the experimental studies for these processes may provide a critical test for different theoretical models.

In this paper, using the multi-configuration Hatree-Fock method with relativistic correction [19], we study numerically the DR cross sections and rate coefficients of a He-like Ar^{16+} in its ground state $1s^2$, through a Ar^{17+} $1s2snl$, $1s2pnl$ (n=2 to 9). The relativistic correction is introduced into the radial equations simply by adding the mass-velocity term and the Darwin term. The self-consistency in the present calculation gets improved. Furthermore, an extrapolation technique is applied to estimate contributions of the very high n complexes. In order to optimize the extrapolation method, the n, l dependence of the DR strengths are investigated, and the contributions of TEOP radiative transitions to the DR cross sections are calculated. Finally, the total and state-to-state DR rate coefficients are presented and analyzed.

2 Theory and computation

In the isolated-resonance approximation, the DR cross sections from initial state i into a final state f through an intermediate doubly excited state d is written as (atomic units are used throughout unless specified) [20]

$$\sigma_{idf} = \frac{\pi^2 \hbar^3}{m_e \varepsilon_{id}} \frac{g_d}{2g_i} \frac{A^a_{di} \cdot A^r_{df}}{\sum\limits_{f'} A^r_{df'} + \sum\limits_{i'} A^a_{di'}} \delta(\varepsilon - \varepsilon_{id}). \tag{2.1}$$

Here m_e is the mass of electron, ε_{id} is the resonance energy, and also the Auger electron energy, g_i and g_d are the statistical weights of the states i and d, respectively, A^a_{di} is the Auger decay rate (inverse resonant capture), which can be calculated by Fermi's golden