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Single and double K-shell vacancy production in N^{7+} + Ti collisions

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Abstract

Non-perturbative classical models were applied in the study of K-shell vacancy production in N^{7+} and Ti collisions in the 4–26 MeV/u projectile energy range. Total cross sections for the single and double K-shell vacancy productions are calculated by means of a simple binary encounter model, classical trajectory Monte–Carlo methods within and beyond the independent electron approximation. The experimental and theoretical ratios of the double- to single-vacancy production yields have been compared. It is demonstrated that a simple model for accounting the final state electron–electron correlation in the double capture and the capture + ionization channels significantly improves the agreement between experiment and theory compared to the independent electron approximation.

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1. Introduction

In the last two decades, considerable interest has been attracted by two-electron transitions like double ionization, double capture, ionization + capture, etc., in atomic collisions. A large amount of experimental work has been performed on He target. Reviews of the topic were made by McGuire [1,2] and McGuire et al. [3]. In many double or multiple transition studies, one should go beyond the independent electron approximation (IEA) [4], and the attention is focused on the role of electron–electron correlation (see e.g. Refs. [5–7]) in the transition. Even for He-like targets, however, it has been shown that IEA approved to be well applicable for the description of double ionization [8] or double charge transfer [9] by bare ion projectiles at high impact velocities.

Double vacancy production in the target K-shell of $Z \geqslant 10$ elements in the high impact energy region is a special case of double transitions. A characteristic feature of the inner shells is that the role of electron correlation in the ground state of the target atom is relatively small. Experimental study of such processes [10–14] can be important for mapping the limits of the applicability of the

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independent electron approximation, which is usually considered to be valid for the inner shell vacancy production process [14–18]. It has been shown that both single and double K to K transfer processes significantly contribute to the K-vacancy production in Ti target if the collision systems are close to the Z_1–Z_2 symmetry [12–14]. It was also shown that perturbative [15,16] and non-perturbative close coupling [17] theoretical models based on IEA provided a general qualitative agreement with experiments.

In the present work our attention is focussed to the vacancy production for the K-shell of titanium. The velocities of the nitrogen projectiles investigated here are in the range of 12–30 a.u. Since $Z_1/Z_2 \sim 0.3$, the relative importance of the charge transfer process is expected to be smaller than in Refs. [11–13]. Single- and double-vacancy production cross sections are calculated, and their ratio is compared with our published and preliminary reported experimental data [10,11]. In all cases, the measurements were performed by the method of X-ray spectroscopy, and the experimental double/single vacancy production ratios were determined from the measured intensity ratios of the K-hypersatellite and K-satellite line groups [10,11].

2. Theoretical method

The calculations were performed by means of different non-perturbative classical models. The simplest one was a classical binary-encounter (i.e., two-body) approximation, the so-called geometrical vacancy-production model [18]. Within this model, the vacancy-production probability at a given impact parameter is identified with a relative fraction of the (normalized) electron density located along the projectile trajectory. This fraction represents electrons which gain a classical energy transfer above an effective threshold level in the binary (projectile–electron) collision. Since only one effective threshold-energy value is used in this simple model, only a total vacancy production probability can be determined. Accordingly, ionization and capture channels cannot be separated. When choosing an effective threshold value, one should keep in mind that the energy transfer depends on the final state of the collision system. Accordingly, the energy transfer values belonging to the capture or excitation processes are typically smaller than the first ionization potential, while the second ionization potential, e.g., is significantly larger. In the present work, as a compromise, the effective threshold energy was taken to be identical to the first ionization potential. The geometrical-model cross-sections were calculated by means of Eq. (17) of Ref. [18]. Of course, this simple model is based on IEA.

At the next level of the present calculations, we applied the four-body classical trajectory Monte-Carlo (CTMC) method [19,20], within the framework of the independent electron approximation. For the present analysis, CTMC calculations has the main advantage that they are non-perturbative, and all the reaction channels can be treated within one theoretical model. Moreover, the role of various interactions can be analyzed in some extent, by neglecting or approximately treating the corresponding potential energy terms in the (classical) Hamiltonian. It makes possible to go beyond IEA. Starting with the simplest assumptions in the first set of the CTMC calculations we performed a four-body calculation by completely neglecting the dynamic e–e interaction term. The considered reactions are:

- single ionization (SI),

$$N^{7+} + Ti \rightarrow N^{7+} + Ti^{+} + e^{-}, \tag{1}$$

- single capture to the projectile bound state (SC),

$$N^{7+} + Ti \rightarrow N^{6+} + Ti^{+}, \tag{2}$$

- double ionization (DI),

$$N^{7+} + Ti \rightarrow N^{7+} + Ti^{2+} + 2e^{-}, \tag{3}$$

- double capture to the projectile bound state (DC), and

$$N^{7+} + Ti \rightarrow N^{5+} + Ti^{2+}, \tag{4}$$

- capture + ionization, where one of the K-shell electrons is captured to the bound state of the projectile and one of them is ejected simultaneously (CI).

$$N^{7+} + Ti \rightarrow N^{6+} + Ti^{2+} + e^{-}. \quad (5)$$

One should note here that the CI process is often referred to as transfer-ionisation (TI) in the literature (see e.g. Refs. [12–14]).

In the present CTMC calculations, Newton's classical non-relativistic equations of motions for a four-body system have been solved numerically for a statistically large number of trajectories for given initial parameters. The four particles of given masses and charges interact with each other via Coulomb forces, except for the two electrons (IEA). The impact parameter of the projectile, the orientation and velocity of the electrons moving around the target nucleus are randomly selected according to the Monte-Carlo method. For taking into account the mean-field component of the electron–electron interaction, at least partially, the binding energies of the two electrons in the Ti atom were chosen as slightly different values of 183 and 188 a.u. The equations of motion were integrated with respect to time as an independent variable by the standard Runge–Kutta method.

The total cross sections for a specific event i are calculated as

$$\sigma_i = \frac{2\pi b_{\max} \sum b_i}{N}, \quad (6)$$

and the standard deviation for a cross section is given by

$$\Delta\sigma_i = \sigma_i \left(\frac{N - N_i}{N N_i} \right)^{1/2}. \quad (7)$$

In Eqs. (6) and (7) N is the total number of trajectories calculated for impact parameters less than $b_{\max}$, N_i is the number of trajectories that satisfies the criteria for the specific event, b_i is the actual impact parameter when the criteria for that event is fulfilled.

At the next step, we performed a second set of CTMC calculations, with replacing the Coulomb forces (approached by appropriate effective Z values) between the target nucleus and the electrons by approximate analytic screened potentials. The two sets of calculations provided the same results within the statistical error limits. Therefore, we concluded that the mean field part of the electron–electron interaction at the target center did not affect the cross sections of the investigated processes significantly.

Finally, we made an attempt to model the fact that the capture of one electron to the projectile center may significantly affect the "history" of the second electron (especially the capture of it) via electron–electron interaction. Within this model, the integration of the IEA four-body trajectories were continued up to the capture of one of the electrons. The condition for the capture was fulfilled when the energy of the electron was negative in the projectile frame and the absolute value of the potential energy term between the electron and the (screened) target nucleus was much smaller (less than 10% – this parameter value was arbitrarily chosen) than that between the electron and the projectile nucleus. It is noted that capture to the 1s shell of the projectile has been found to be dominant by the calculations, and the result were practically not sensitive on the value of the above free parameter within some reasonable limits (5–15%).

Once one of the electrons was captured, we applied a sudden change in the calculation. The captured electron was frozen to the projectile nucleus as a 1s-type screening cloud, and we continued with a three-body calculation for the trajectory of the other electron. In the following, this method will be referred to as *frozen-electron calculation*. This way, we roughly modeled a repulsive force between the two electrons when they both approach the same (projectile) center during the evolution of the final state. If our picture is correct, even this simple model should add a correction to IEA in a good direction.

Obviously, pure ionization channels (SI and DI) remain unchanged, and only the SC, DC and CI reaction channels are modified by the above model. In the following, the corresponding theoretical results will be denoted by SC–F, DC–F, and CI–F, respectively. In general, these frozen–electron CTMC calculations will be referred to as CTMCF.

3. Results and discussion

Fig. 1 shows the single (part a) and double (part b) K-vacancy production cross sections as a function of the impact energy. As it can be seen, the shape of the curves obtained by the CTMC and CTMCF methods and the geometrical model (GM) are similar, but there are big differences in the absolute values. The geometrical model predicts much smaller vacancy production cross sections than either of the CTMC calculations. One should note here that the cross sections obtained from the geometrical model are only by 10–20% larger than those calculated in the framework of semiclassical approximation for the pure ionization contribution, performed by the authors (not shown in the figure). The charge transfer channel seems to be strongly underestimated by the geometrical model compared to CTMC or CTMCF.

A more detailed analysis of the various contributions to the single and double K-shell vacancy production is provided in Fig. 2. The different energy-dependence of the ionization and the capture components is obvious. It is also clear that the frozen-electron results are higher than the IEA result for SC, but they are significantly smaller

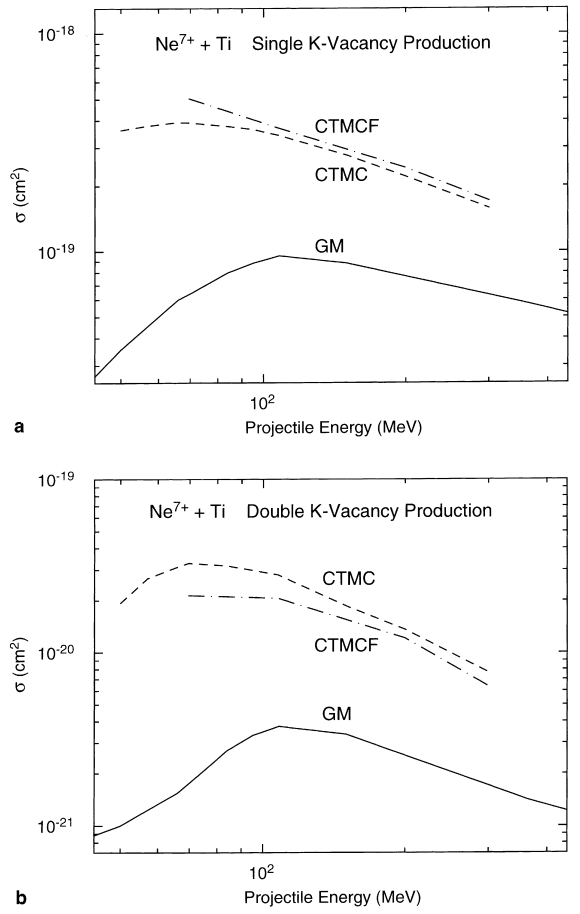

Fig. 1. Calculated cross sections for single (a) and double (b) vacancy production in N^{7+} + Ti collisions. Dashed lines: CTMC calculations within the IEA framework; dashed-dotted lines: CTMCF calculations; solid line: GM results.

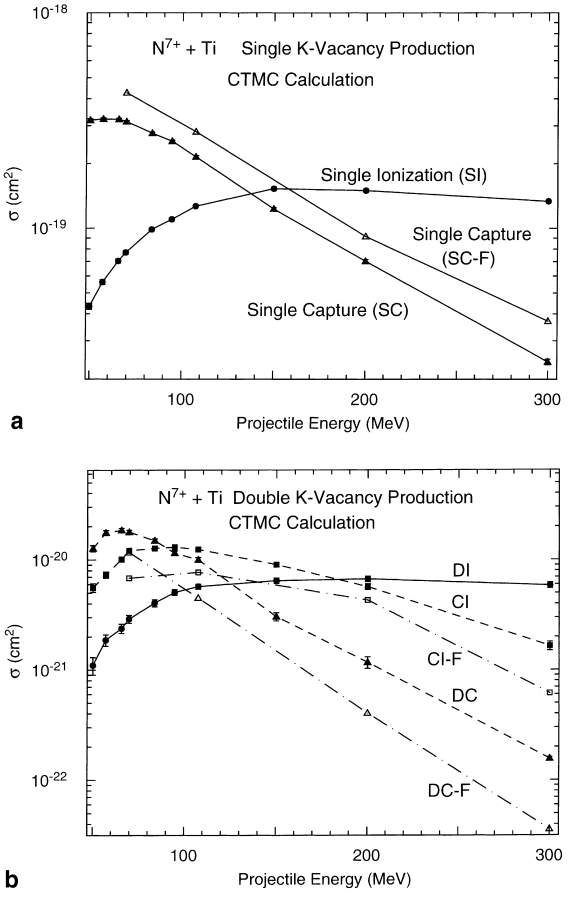

Fig. 2. Calculated cross sections for the various reaction channels for single (a) and double (b) vacancy-production in N^{7+} + Ti collisions by CTMC and CTMCF methods. The abbreviations are listed in the text. Notice the differences between the independent electron approximation and the frozen-electron model results.

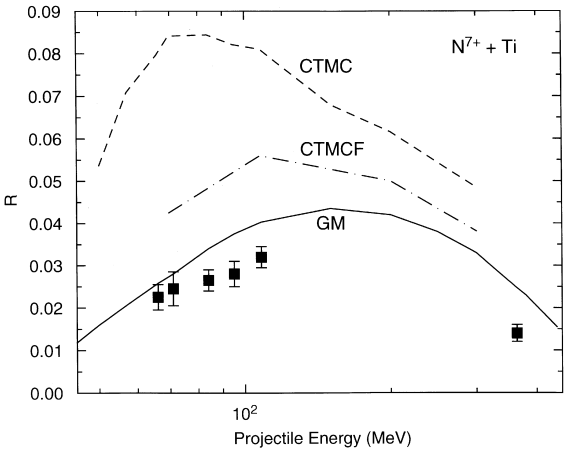

Fig. 3. Ratio of double- to single-vacancy production cross sections. Dashed line: CTMC; dashed-dotted line: CTMCF; solid line: GM; full symbols: experiment.

than the IEA results for both double transitions including capture (DC and CI).

Finally, Fig. 3 displays the theoretically obtained ratios of double- to single-vacancy production cross sections in comparison with the experimental data. Although the geometrical model is a very simple two-body approximation, the values are closer to the experimental data than that of CTMC or CTMCF. Especially the CTMC (IEA) ratios are much (about three times) higher than the experimental data. In this approximation the ratio of the single to double K-shell vacancy production $[R = (\mathrm{DI+DC+CI})/(\mathrm{SI+SC})]$ varies between 7.8% and 8.4% in the impact energy range of 4.7–7.71 MeV/u. The corresponding experimental results vary between 2.25% and 3.2% [10,11]. The ratios calculated by the CTMCF model are much closer to the measured ratios than those calculated by the four-body CTMC method within IEA. The frozen–electron model seems to give account of a real effect, namely the significant role of electron–electron correlation in the final state when the electrons approach the projectile nucleus.

The relatively better agreement with the results of the geometrical model also shows that the intensity of the charge transfer processes is probably overestimated by the CTMC calculation, especially the DC and the CI channels. CTMCF calculations qualitatively show that the discrepancy can be attributed to the neglect of the *final-state* electron–electron interaction in the CTMC calculations. It seems to be surprising that IEA was found to be applicable for the description of the double capture process in He^{2+} + He collisions [9].

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