# Dielectronic recombination of Ni-like ions through the $3d^9 4ln'l'$ ($n'=4,5$) Cu-like configurations

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*Ab initio* calculations of the rate coefficients for dielectronic recombination (DR) of ten ions along the Ni I isoelectronic sequence in the ground state ($Mo^{14+}$, $Ag^{19+}$, $Xe^{26+}$, $Pr^{31+}$, $Gd^{36+}$, $Dy^{38+}$, $Ta^{45+}$, $Au^{51+}$, $At^{57+}$, and $U^{64+}$) through the Cu-like $3d^9 4ln'l'$ ($n'=4,5$) inner-shell excited configurations were performed using the HULLAC code package. Resonant and nonresonant radiative stabilizing transitions and decays to autoionizing levels followed by radiative cascades are included. Collisional transitions following electron capture are neglected. Nonresonant stabilizing transitions are found to enhance the DR rates, and may even dominate the process at low electron temperature. The remarkable difference between the isoelectronic trend of the rate coefficients for DR through $3d^9 4l4l'$ and through $3d^9 4l5l'$ is emphasized. The trend of DR through $3d^9 4l4l'$ shows irregularities at relatively low temperature due to the progressive closing of DR channels as $Z$ increases. Thus, the DR coefficients cannot be reproduced or interpolated by a simple analytical formula. Even for the smooth contributions of the $3d^9 4l5l'$ configurations, a simplified model using configuration averaging for autoionization and radiative decays instead of level-by-level detailed computations is found to overestimate the DR rates by a factor of up to 2.

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## I. INTRODUCTION

The knowledge of accurate ionization and recombination rates of heavy ions is crucial for the study of ionization balance of highly ionized elements in hot plasmas (see, for instance, Refs. [1,2]). This knowledge is also important for the research of x-ray lasers, specifically for calculating the populating and depopulating of lasing levels [3,4]. In a previous work [5] the contribution of excitation-autoionization (EA) processes to the total ionization for heavy Cu-like to Kr-like ions was computed and the relative effect of EA on the ion abundances in coronal plasmas was thoroughly studied. It was found that the position of $3d$-inner-shell excited configurations is above or below the ionization limit depending on the atomic number $Z$. Therefore the contribution of these configurations to EA can vary drastically along a given isoelectronic sequence. In order to complete the accurate ionization balancing, precise data on recombination rates are needed. The main recombination process in highly ionized plasmas is the dielectronic recombination (DR).

In the present work, we focus on DR for ions of the Ni I isoelectronic sequence in the ground state. Previous works on this sequence were performed only for $Gd^{36+}$ [6] and $Ta^{45+}$ [7]. Unfortunately, the strong variation of the DR rate coefficients along the sequence makes extrapolation or interpolation within the sequence inaccurate. Moreover, the general semiempirical Burgess-Merts formula [8,9] for DR coefficients was found to overestimate the total coefficients for heavy highly ionized elements [6]. Thus in the present work extensive detailed *ab initio* calculations for the different elements along the sequence have been performed. The two Cu-like configuration complexes $3d^9 4l4l'$ and $3d^9 4l5l'$, which are expected to give the strongest contributions to DR, are considered here. All calculations are performed assuming no collisional transitions occur after the initial electron capture.

The importance of radiative cascades through lower autoionizing levels in the DR process has been previously pointed out for sequences isoelectronic to light elements by Gau, Hahn, and Retter (e.g., Ref. [10]). According to those calculations performed in the $LS$ coupling scheme, these processes can reduce the DR rates of $Mo^{32+}$ by as much as 30%. Nevertheless, in more recent works [6,7,11] (where a more adequate relativistic code was used) cascades were neglected, and also only the resonant radiative transitions were considered. Since in the Cu I isoelectronic sequence some inner-shell excited levels (of the $3d^9 4l4l'$ configuration complex) lie below the ionization limit, nonresonant decays from the autoionizing levels towards these levels constitute a stabilizing channel for the effective DR process, and thus might be of significant importance to the DR rates. In the present work, these nonresonant stabilizing transitions have been included and their contribution investigated, together with the effect of decays to autoionizing levels followed by cascades.

In this study, one has to distinguish between the isoelectronic behavior of DR through the inner-shell excited levels of the $3d^9 4l4l'$ configuration complex lying close to the first ionization limit, and the isoelectronic behavior of DR through higher lying levels, such as those from the $3d^9 4l5l'$ configuration complex. The contribution of the

 

$3d^94l4l'$ configuration complex is expected to vary irregularly from element to element along the sequence, as was observed for EA processes, since the number of levels from these configurations which lie above the first ionization limit varies along the sequence. In this complex a single level lying above but very close to the ionization limit might strongly enhance and even dominate the whole DR process at low electron temperature. Such peculiar levels are of special interest for the research of x-ray lasers, since strong captures to particular inner-shell excited levels may lead to population inversion and a lasing process.

On the other hand, one expects the $3d^94l5l'$ configuration complex to give a smooth contribution to DR along the Ni I sequence, which is typical of high lying configurations. This contribution becomes very significant at high electron temperature. The more regular isoelectronic trend for these configurations, along with the very large number of levels and computations involved in obtaining total DR rates, motivate the development of approximate methods. A configuration averaging method proposed by Bauche-Arnoult *et al.* [12] is tested herein on particular configurations, and the validity of the method is discussed.

## II. THEORETICAL METHOD

In this work, the dielectronic recombination of a Ni-like ion in its ground state $3d^{10}$, through a Cu-like $3d^94ln'l'$ ($n'=4,5$) inner-shell excited level lying above the ionization limit, to any final state below the ionization limit is considered. This process can be schematically represented by

$$[\text{Ar core}]3d^{10}+e^- \leftrightarrow [\text{Ar core}]3d^94ln'l' \quad (n'=4,5), \tag{1}$$

$$[\text{Ar core}]3d^94ln'l' \rightarrow [\text{Ar core}]3d^{10}n''l''+h\nu, \tag{2a}$$

or

$$[\text{Ar core}]3d^94ln'l' \rightarrow [\text{Ar core}]3d^94l4l''+h\nu, \tag{2b}$$

where [Ar core]$3d^{10}$ represents a Ni-like ion, [Ar core] symbolizing the full $1s^22s^22p^63s^23p^6$ electronic inner shells. $e^-$ is the interacting free electron and $h\nu$ the emitted photon. The first process is the electron capture which is reversible by autoionization, whereas processes (2a) and (2b) are the resonant and nonresonant radiative stabilizing transitions, respectively. Nonresonant stabilizing transitions [process (2b)] refer to radiative decays from autoionizing levels to inner-shell excited levels below the ionization limit. In cases where the radiative decay from the $3d^94ln'l'$ level is to another inner-shell excited level above the ionization limit, the stabilization [via either (2a) or (2b)] can be reached after several consecutive radiative transitions (cascades).

The rate coefficient $\beta_{kd}$ for process (1) only, i.e., the capture of a free electron by a Ni-like ion in its ground state $k$, to form a Cu-like ion in an excited state $d$ above the first ionization limit, can be evaluated by the principle of detailed balance. Assuming a Maxwellian electron velocity distribution corresponding to an electron temperature $T_e$, one obtains for the capture rate coefficient (see, for instance, Ref. [13])

$$\beta_{kd}=1.656\times10^{-22}(kT_e)^{-3/2}\frac{g_d}{g_k}A^a_{dk}\exp\left(\frac{-\Delta E_d}{kT_e}\right), \tag{3}$$

where $\Delta E_d$ is the energy difference between the level $d$ and the ionization limit. $\Delta E_d$ and $kT_e$ are expressed in eV. $A^a_{dk}$ is the coefficient for autoionization from level $d$ to $k$, expressed in $s^{-1}$. $g_d$ and $g_k$ are the statistical weights of the $d$ and $k$ levels, respectively. $\beta_{kd}$ is expressed in cm$^3$ s$^{-1}$.

Neglecting electron collision processes for depletion of excited levels, the inner-shell excited Cu-like ion in level $d$ can either autoionize back to a Ni-like ion or decay radiatively. This decay can be towards a level $d'$ above the ionization limit ($k$) from which it can further either autoionize or decay, or it can be to a level $i$ or $d''$ below the ionization limit (i.e., effective recombination); $i$ denotes a $3d^{10}n''l''$ level of the recombined Cu-like ion [reaction (2a)], and $d''$ a $3d^94l4l''$ level below the ionization limit [reaction (2b)]. Thus, considering all these possible processes from level $d$, the multiple branching ratio for (effective) dielectronic recombination through a level $d$ can be defined recursively:

$$B^D(d)=\frac{\sum_i A_{di}+\sum_{d''<k}A_{dd''}+\sum_{d'>k}A_{dd'}B^D(d')}{\sum_{k'}A^a_{dk'}+\sum_i A_{di}+\sum_{d''<k}A_{dd''}+\sum_{d'>k}A_{dd'}}. \tag{4}$$

$\Sigma A_{di}$, $\Sigma A_{dd''}$, and $\Sigma A_{dd'}$ are the sums of the Einstein coefficients for spontaneous emission from level $d$ to levels $i$, $d''$, and $d'$, respectively. $\Sigma A^a_{dk'}$ is the total coefficient for autoionization from level $d$ to any level $k'$ of the Ni-like ion.

In this work, the most important $3d^94ln'l'\rightarrow3d^94l4l''$ and $3d^94ln'l'\rightarrow3d^{10}n''l''$ electric dipole radiative decays have been considered; however, $3d^94l5l'\rightarrow3d^94l5l''$ radiative transitions have been neglected. Totally neglecting both nonresonant stabilizing transitions and cascades through autoionizing levels reduces the branching ratio for recombination given by Eq. (4) to the commonly used approximate form:

$$B^D(d)\approx\frac{\sum_i A_{di}}{\sum_{k'}A^a_{dk'}+\sum_i A_{di}}. \tag{4$'$}$$

The $\Sigma A^a_{dk'}$ sum in Eqs. (4) and (4$'$) reduces in most cases to one single term $A^a_{dk}$: the autoionization to the ground state $3d^{10}$. Autoionization to the $3d^94l$ excited levels of the Ni-like ion, which might reduce the DR rates [14], is not relevant for the intermediate configurations considered here for $Z>47$, since all the inner-shell excited levels of these ions have energies lower than the $3d^94s$ levels. However, for the Mo to Ag ions the autoionization from some upper levels of $3d^94f5f$ and $3d^94f5g$ to $3d^94s$ and $3d^94p$ levels is energetically possible and has been taken into account in this work.

The rate coefficient for effective DR, i.e., for process (1) plus processes (2a) and (2b), from the initial ground level $k$ of the Ni-like ion through a given intermediate level $d$ of a Cu-like $3d^9 4ln'l'$ inner-shell excited configurations, to any final nonautoionizing level $i$ or $d''$ of the Cu-like ion is given by

$$\alpha_{kd}^D = \beta_{kd} B^D(d). \tag{5}$$

The total rate coefficient for DR from the initial level $k$ is finally given by summing over all possible $d$ levels within each inner-shell excited configuration:

$$\alpha_k^D = \sum_d \alpha_{kd}^D. \tag{6}$$

An approach alternative to the branching ratio method is the transition-rate matrix formalism presented by Jacobs and Blaha [15], which is a collisional-radiative model for describing the population distribution among the autoionizing levels. This matrix method is the appropriate tool for analyzing dielectronic spectra, since it relates the whole DR process to the final radiative decay. Moreover, in high density plasmas, where collisional processes between autoionizing levels have to be included, the presently employed branching ratio formalism is inapplicable. However, for the purpose of total recombination rate calculations when collisions following the initial electron capture can be ignored, the branching ratio formalism is more adequate, and is in fact the straightforward approach. When thousands of levels have to be included, such as in the present work, it is simpler to deal with each primary capture process independently, and not complicate the computations by crossconnecting all the individual levels. The branching ratio method is therefore appropriate for calculating DR rates for complex configurations in many-electron sequences.

It should be stressed that in a model where the recombination consists of an electron capture followed by a *single* radiative decay, and cascades (radiative or collisional) are negligible, the two approaches are equivalent. In this case the transition-rate matrix is diagonal, and its diagonal elements are none other than the denominators of the branching ratios for the different autoionizing levels.

The detailed level energies and radiative decay coefficients were computed here using the multiconfiguration relativistic RELAC code [16]. The autoionization coefficients were calculated in the semirelativistic distorted-wave approximation using the factorization-interpolation model implemented in the HULLAC code package [17]. This method has been described in detail in Ref. [17], and has been applied in many cases and successfully tested by comparison to other calculation methods [17,18].

## III. CALCULATIONS

In the following the main features of the computations performed using detailed level-by-level calculations for ten elements, Mo ($Z=42$), Ag (47), Xe (54), Pr (59), Gd (64), Dy (66), Ta (73), Au (79), At (85), and U (92), along the Ni I isoelectronic sequence are presented, and their importance is discussed.

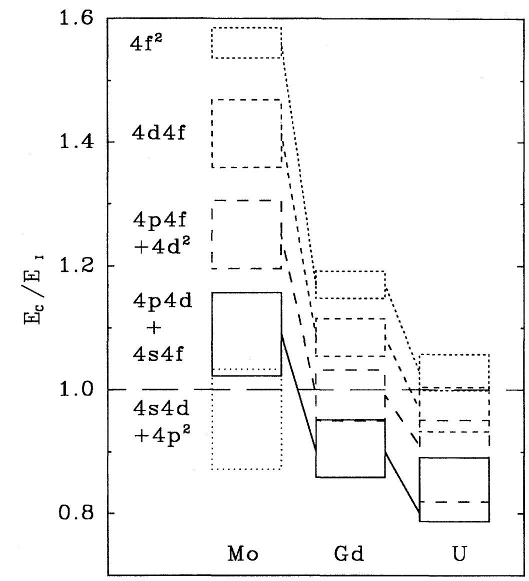


FIG. 1. Energy $E_c$ of the inner-shell excited configurations within the $3d^9 4l4l'$ complex relative to the first ionization limit $E_I$ for three elements in the Cu I isoelectronic sequence. For the $Gd^{35+}$ and $U^{63+}$ Cu-like ions the $3d^9[4s4d+4p^2]$ mixed configurations are well below the ionization limit, and are not plotted. The energies are indicated by a finite vertical range representing the full level spread within each configuration.

### A. Closing of DR channels

Figure 1 shows the energy spread of the configurations pertaining to the Cu-like $3d^9 4l4l'$ complex which may contribute to DR of Ni-like ions for three elements: Mo, Gd, and U. The configuration energies $E_c$ are plotted relative to the first ionization limit $E_I$ of the same ion. As the atomic number $Z$ increases along the isoelectronic sequence, fewer levels of the complex contribute to DR, due to the lowering of the energy levels and thus the closing of DR channels. The $3d^9 4s^2$ and $3d^9 4s4p$ configurations which lie below the ionization limit for all the elements considered are not represented in the figure. For $Mo^{14+}$, the $3d^9[4s4d+4p^2]$ mixed configurations contribute to DR, whereas for the two other elements they lie below the ionization limit (and are also not shown in the figure). For $U^{64+}$ only the $3d^9 4d4f$ and $3d^9 4f^2$ configurations out of the whole complex still contribute.

This trend is well reflected in Table I. This table displays the results of the detailed computations for the rate coefficients for DR through the various configurations within the $3d^9 4l4l'$ complex (including nonresonant transitions and cascades) at $kT_e = 200$ eV for the ten Ni-like ions considered. The second column gives the number of levels lying above the first ionization limit, out of the 685 levels of the whole configuration complex. The following columns display the contributions of the different configurations to the DR rate coefficient, and directly reflect the effect of the progressive closing of the DR channels as $Z$ increases. This isoelectronic behavior can be correctly reproduced only by detailed level-by-level calculations.

TABLE I. Contribution of the various Cu-like configurations within the $3d^94l4l'$ complex to the total DR rate coefficient for ten ions of the Ni I isoelectronic sequence at $kT_e=200$ eV. $N$ is the number of autoionizing levels out of the 685 levels of the complex. The rate coefficients are given in cm$^3$ s$^{-1}$. $X[-Y]$ denotes $X\times10^{-Y}$.

| Ion | $N$ | $3d^9[4s4d+4p^2]$ | $3d^9[4p4d+4s4f]$ | $3d^9[4p4f+4d^2]$ | $3d^94d4f$ | $3d^94f^2$ |
|---|---|---|---|---|---|---|
| $Mo^{14+}$ | 599 | 2.14[−14] | 3.66[−12] | 5.16[−12] | 4.28[−12] | 3.30[−12] |
| $Ag^{19+}$ | 552 | 0 | 6.54[−12] | 1.35[−11] | 1.21[−11] | 8.71[−12] |
| $Xe^{26+}$ | 468 | | 1.08[−11] | 3.70[−11] | 3.05[−11] | 2.10[−11] |
| $Pr^{31+}$ | 440 | | 0 | 6.88[−11] | 5.20[−11] | 3.43[−11] |
| $Gd^{36+}$ | 340 | | | 7.30[−11] | 8.24[−11] | 5.38[−11] |
| $Dy^{38+}$ | 314 | | | 7.35[−11] | 9.67[−11] | 6.33[−11] |
| $Ta^{45+}$ | 283 | | | 0 | 1.68[−10] | 1.09[−10] |
| $Au^{51+}$ | 192 | | | | 2.66[−10] | 1.66[−10] |
| $At^{57+}$ | 161 | | | | 3.13[−10] | 2.59[−10] |
| $U^{64+}$ | 115 | | | | 2.10[−10] | 4.58[−10] |

### B. Configuration mixing

In the $3d^94l4l'$ case the configuration interaction (CI) cannot be neglected. Particularly important are the interactions between $3d^94s4d$ and $3d^94p^2$, $3d^94p4d$ and $3d^94s4f$, and $3d^94p4f$ and $3d^94d^2$ [19]. For this reason the summed coefficients for DR through the mixed configurations are given in these cases. An illustration of the significance of these configuration mixings is given in Table II. This table shows a comparison between calculations performed in the model of the isolated configurations approximation (IS), and computations including CI, for $Gd^{36+}$ at $kT_e=100$ and 1000 eV. In the CI case the summed rate coefficient for DR through the $3d^9[4p4f+4d^2]$ mixed configurations is given. In both cases, only resonant radiative transitions were considered in order to simplify the calculations.

It is shown for both temperatures that DR through the $3d^9[4p4f+4d^2]$ mixed configurations is more than six times stronger than DR through both isolated configurations in the IS model. Moreover, at low electron temperature the contribution of these two configurations within the $3d^94l4l'$ complex becomes dominant. Thus at 100 eV the mixing enhances the total rate for DR through the whole complex by almost a factor of 2 (Table II).

This strong effect is explained by the mixing of a configuration which is strongly autoionizing ($3d^94d^2$) with a configuration which has a strong resonant radiative decay ($3d^94p4f$), since the rate coefficient for effective DR for each level $d$ is proportional (in this resonant transition decay approximation) to the product of $A^a_{dk}$ and $\Sigma A_{di}$ [Eqs. (3), (4′), and (5)]. Although detailed level-by-level computations have been performed, a qualitative picture of this effect can be directly obtained by evaluating the sum of the autoionization coefficients $\Sigma_d A^a_{dk}$ and the radiative coefficients $\Sigma_d\Sigma_i A_{di}$ over the whole configuration. In the IS model the term $\Sigma A^a$ for the $3d^94d^2$ configuration has a high value of $2.1\times10^{15}$ s$^{-1}$, whereas $\Sigma\Sigma A$ for electric dipole transitions is zero, since the $4d\rightarrow3d$ transition is optically forbidden. For the $3d^94p4f$ configuration, summing over all levels one obtains in this model $\Sigma A^a=2.3\times10^{14}$ s$^{-1}$ and $\Sigma\Sigma A=5.8\times10^{14}$ s$^{-1}$. However, in the CI model the $3d^9[4p4f+4d^2]$ mixed configurations have simultaneously high values for both the $\Sigma A^a$ and $\Sigma\Sigma A$ terms ($2.35\times10^{15}$ and $6.12\times10^{14}$ s$^{-1}$, respectively), leading to a strong DR effect.

The influence of configuration mixing on the DR rates has been checked for the $3d^94l5l'$ configuration complex as well, and was found to be much less crucial than for the $3d^94l4l'$ complex. Considering, for instance, the $Gd^{36+}$ ion, one finds that the rate coefficient for DR through the mixed configurations $3d^9[4p5f+4d5d]$ in the CI model is larger than the rate coefficient for the two isolated $3d^94p5f$ and $3d^94d5d$ configurations in the IS model by only 8%.

### C. Nonresonant stabilizing transitions and decays to autoionizing levels

In the course of this study it was found that the best way to take the additional effects in the DR process included in this section into account was to divide them into two parts:

TABLE II. Rate coefficients (in cm$^3$ s$^{-1}$) for DR through the various Cu-like configurations within the $3d^94l4l'$ complex for $Gd^{+36}$ at $kT_e=100$ and 1000 eV calculated in the isolated configurations approximation (IS), compared to the results of configuration interaction (CI) calculations. In the CI model the DR coefficients for the $3d^9[4p4f+4d^2]$ mixed configurations are given. $X[-Y]$ denotes $X\times10^{-Y}$.

| $T_e$ (eV) | Model | $3d^94p4f$ | $3d^94d^2$ | $3d^94d4f$ | $3d^94f^2$ | Total $3d^94l4l'$ |
|---|---|---|---|---|---|---|
| 100 | IS | 2.50[−11] | 0 | 1.03[−10] | 3.89[−11] | 1.67[−10] |
| | CI | 1.63[−10] | | 1.02[−10] | 3.75[−11] | 3.02[−10] |
| 1000 | IS | 1.10[−12] | 0 | 1.28[−11] | 1.48[−11] | 2.87[−11] |
| | CI | 7.10[−12] | | 1.26[−11] | 1.43[−11] | 3.30[−11] |

TABLE III. Ratios of the rate coefficients for DR through the $3d^94ln'l'$ ($n'=4,5$) complexes calculated including NRS and DAC processes to coefficients obtained by taking into account resonant transitions only. For each ion the first line displays the results including NRS and the second line the total results including NRS and DAC.

| Ion | | $T_e$ 10 eV | 20 eV | 100 eV | 1000 eV | 10 000 eV |
|---|---|---|---|---|---|---|
| | | | $3d^94l4l'$ complex | | | |
| $Mo^{14+}$ | NRS | 2.48 | 1.78 | 1.16 | 1.08 | 1.08 |
| | NRS+DAC | 2.50 | 1.86 | 1.30 | 1.19 | 1.19 |
| $Pr^{31+}$ | NRS | 1.47 | 1.25 | 1.08 | 1.03 | 1.03 |
| | NRS+DAC | 1.47 | 1.25 | 1.09 | 1.05 | 1.05 |
| $Gd^{36+}$ | NRS | 1.36 | 1.15 | 1.06 | 1.03 | 1.03 |
| | NRS+DAC | 1.36 | 1.15 | 1.07 | 1.04 | 1.04 |
| $Ta^{45+}$ | NRS | 1.75 | 1.30 | 1.07 | 1.03 | 1.03 |
| | NRS+DAC | 1.75 | 1.30 | 1.07 | 1.04 | 1.03 |
| $U^{64+}$ | NRS | 1.04 | 1.03 | 1.02 | 1.02 | 1.02 |
| | NRS+DAC | 1.04 | 1.02 | 1.02 | 1.02 | 1.02 |
| | | | $3d^94l5l'$ complex | | | |
| $Mo^{14+}$ | NRS | 10.82 | 3.32 | 1.26 | 1.15 | 1.14 |
| | NRS+DAC | 10.94 | 3.61 | 1.45 | 1.25 | 1.24 |
| $Pr^{31+}$ | NRS | 18.86 | 5.11 | 1.76 | 1.13 | 1.11 |
| | NRS+DAC | 18.86 | 5.11 | 1.85 | 1.20 | 1.16 |
| $Gd^{36+}$ | NRS | 32.45 | 6.72 | 2.01 | 1.21 | 1.17 |
| | NRS+DAC | 32.45 | 6.72 | 2.01 | 1.23 | 1.20 |
| $Ta^{45+}$ | NRS | 45.58 | 16.11 | 2.13 | 1.21 | 1.17 |
| | NRS+DAC | 45.58 | 16.11 | 2.14 | 1.24 | 1.19 |
| $U^{64+}$ | NRS | 69.30 | 4.46 | 1.44 | 1.26 | 1.21 |
| | NRS+DAC | 69.30 | 4.46 | 1.44 | 1.25 | 1.19 |

*nonresonant stabilizing* transitions (NRS) on one hand, and *decays* to *autoionizing* levels possibly followed by radiative *cascades* (DAC) on the other. Nonresonant stabilizing transitions are radiative decays from autoionizing levels, where the electron capture occurs, to inner-shell excited levels lying below the ionization limit. The NRS transitions increase the effective DR rates. On the other hand, radiative decays to autoionizing levels may increase or decrease the effective DR, depending on the relative importance of the further radiative decay processes compared to the autoionization processes from these intermediate levels. It has been found here that the NRS can enhance the DR rates very significantly, and this effect is dominant over the DAC. This is due to the relatively large number of nonautoionizing inner-shell excited configurations in the Cu I sequence.

The relative effect of NRS and DAC on the rate coefficients for DR through the two considered complexes is shown in Table III. The first line for each ion in the table gives the ratio between the DR rates obtained by including NRS (but neglecting DAC) and the DR rates obtained by taking only the resonant transitions into account. For each ion the second line gives the total relative DR rates obtained by including also the effect of DAC, in addition to the NRS. Results are presented here for five ions from which the trend of the whole isoelectronic sequence can be deduced.

The varying importance of these effects can be interpreted as follows: In the $3d^94l5l'$ complex the NRS effect is strong, although the coefficients for radiative transitions filling the open $3d$ inner shell (referred to here as resonant transitions) are larger than the coefficients for any other type of (nonresonant) radiative transition. This is due to the large number of decay channels to nonautoionizing low levels within the $3d^94l4l'$ complex, and especially to the significant contribution of nonresonant decays from those $3d^94l5l'$ configurations which have no direct electric dipole transition to the $3d^{10}n''l''$ configurations (for example, $3d^94d5s$ and $3d^94d5g$). At very low electron temperature the contribution of DR via NRS even completely dominates the DR through this complex, because of the NRS decays from low lying configurations of the complex, such as $3d^94s5s$ and $3d^94s5d$. These configurations, especially in high-$Z$ ions, lie just above the ionization limit, and thus give the dominant contributions to the DR at low electron temperature via nonresonant decays solely. It should be stressed that at low electron temperature, even with the strong NRS effect, the contribution of the whole $3d^94l5l'$ complex is still much smaller than the contribution of the $3d^94l4l'$ complex (Tables V and VI). At higher electron temperature, where the contribution of the $3d^94l5l'$ complex becomes important, all NRS decays from this complex still enhance the DR through the whole complex by about 20%. This effect is approximately constant throughout the whole isoelectronic sequence.

In the $3d^94l4l'$ complex the effect of NRS is not as strong for two major reasons: first, the $\Delta n=0$ NRS decays ($4l'\rightarrow 4l''$) are even weaker than the $\Delta n=1$ NRS decays ($5l'\rightarrow 4l''$) from the $3d^94l5l'$ complex, in comparison to the strong resonant $nl' \rightarrow 3d$ transitions. Second, most of the levels in this complex, which have no direct electric dipole transition to the $3d^{10}n''l''$ configurations, and otherwise could have given a strong indirect contribution, lie below the ionization limit, especially for the high-$Z$ ions. This second fact is clearly observed through the isoelectronic trend within the $3d^9 4l4l'$ complex. As $Z$ increases, the number of levels of this kind which lie above the ionization limit decreases (Fig. 1). This gradually reduces the significance of the NRS contribution to DR for the heavier ions. Therefore the effect of NRS decreases along the sequence as $Z$ increases (Table III). The strong out-of-trend enhancement of DR through this complex by NRS for tantalum at low temperature is due to the relatively moderate rates of DR via resonant transitions, and not to a peculiar NRS effect. This has to do with the fact that there is no inner-shell excited level lying just above the ionization limit as exists for other ions (see Sec. IV A). Thus the irregular strong ratios for tantalum appearing in Table III can be understood by the fact that only the *relative* NRS effect compared to the resonant transitions approximation is shown. For $Z > 72$ the calculations show that the effect of NRS in the $3d^9 4l4l'$ complex is less than 5% for all electron temperatures, because only the $3d^9 4d4f$ and $3d^9 4f^2$ configurations, from which resonant decay is very strong, are above the ionization limit. On the other hand, for the relatively light ions, especially at low electron temperature, there is a significant relative effect of up to a factor of 2.5 (for Mo at 10 eV) in this complex; this obviously cannot be neglected, since at low temperature the contribution of this complex to the total DR rates is predominant.

The effect of DAC processes can be seen in the second line for each ion in Table III, where the total relative DR rates obtained by including both NRS and DAC processes are given. The DAC effect appears to be mostly in the same direction as the NRS effect, but is generally much less important. The DAC processes are found to be noticeable only for the relatively light ions. For the heavier ions most of the $3d^9 4l4l'$ levels, which are the lower levels of the nonresonant transitions from both $3d^9 4ln'l'$ complexes, lie below the ionization limit; this leaves very few decay channels through autoionizing levels. The relative importance of DAC rises at high electron temperature, where the population of the upper levels allows for decays to autoionizing levels; this holds for both complexes, as can be seen in Table III.

Altogether the DAC effect remains very limited (generally less than 10%), if not completely negligible along the whole isoelectronic sequence. This can be understood by analyzing the changes in the branching ratio for recombination. Including DAC means adding the term $\Sigma A_{dd'} B^D(d')$ to the numerator and the term $\Sigma A_{dd'}$ to the denominator of the branching ratio for recombination [see Eq. (4)]. On the average, assuming that this branching ratio for the different levels is more or less constant, this adjustment should have no influence, because in this approximation the term added to the numerator is smaller than the term added to the denominator by the same ratio as the original ratio $B^D(d)$. Thus the effect of DAC has to be a consequence of deviations from this averaging behavior. This simple fact justifies our definition of the NRS approximation, where we have completely disregarded decays to autoionizing levels by omitting these transitions both in the numerator and in the denominator of the branching ratio.

For the relatively low-$Z$ ions, the branching ratios for recombination are usually much smaller than unity, since the autoionization coefficients $A^a$ are much larger than the radiative coefficients $A$. Therefore the branching ratios for these ions are more sensitive to the minor DAC correction terms; this fact is directly reflected in the noticeable change appearing in the DR rates of these ions (Table III). For the heavy elements, the radiative coefficients are of the same order of magnitude or even larger than the autoionization coefficients, and thus the DR rates of the heavy ions are less affected by DAC.

The clear conclusion from the present results is that accurate calculations of rate coefficients for DR of Ni-like ions at any temperature must take into account the nonresonant stabilizing transitions, whereas the DAC contribution gives a rather small correction and may be neglected for most applications.

### D. Average methods

In a previous work [12] configuration averaging methods for computing DR rate coefficients were proposed for mod-

TABLE IV. Average quantities used for the computation of $\overline{\alpha_c^D}$ for the $3d^9 4f5f$ configuration (second through sixth columns). The sixth and eighth columns show the sum terms appearing in the expressions of $\overline{\alpha_c^D}$ and $\alpha_c^D$, respectively. The final rate coefficients $\overline{\alpha_c^D}$ and $\alpha_c^D$ at $kT_e = 1$ keV are given in the seventh and ninth columns, respectively. $X[-Y]$ denotes $X \times 10^{-Y}$.

| Ion | $\overline{\Delta E_c}$ (eV) | $\Sigma\Sigma A$ ($s^{-1}$) | $\Sigma\Sigma A^a$ ($s^{-1}$) | $\Sigma g A^a$ ($s^{-1}$) | $\frac{(\Sigma g A^a)(\Sigma\Sigma A)}{\Sigma\Sigma A^a + \Sigma\Sigma A}$ ($s^{-1}$) | $\overline{\alpha_c^D}$ (1 keV) ($cm^3\ s^{-1}$) | $\Sigma \frac{g A^a \Sigma A}{\Sigma A^a + \Sigma A}$ ($s^{-1}$) | $\alpha_c^D$ (1 keV) ($cm^3\ s^{-1}$) |
|---|---|---|---|---|---|---|---|---|
| $Mo^{14+}$ | 226 | 6.06[13] | 1.72[15] | 5.98[15] | 2.04[14] | 8.51[−13] | 2.12[14] | 8.75[−13] |
| $Ag^{19+}$ | 318 | 1.92[14] | 1.17[15] | 1.02[16] | 1.43[15] | 5.45[−12] | 8.31[14] | 3.12[−12] |
| $Xe^{26+}$ | 456 | 5.96[14] | 1.70[15] | 1.46[16] | 3.79[15] | 1.26[−11] | 2.23[15] | 7.23[−12] |
| $Pr^{31+}$ | 560 | 1.10[15] | 1.99[15] | 1.71[16] | 6.07[15] | 1.82[−11] | 3.65[15] | 1.06[−11] |
| $Gd^{36+}$ | 672 | 1.87[15] | 2.21[15] | 1.89[16] | 8.63[15] | 2.31[−11] | 5.37[15] | 1.39[−11] |
| $Dy^{38+}$ | 718 | 2.26[15] | 2.30[15] | 1.96[16] | 9.71[15] | 2.48[−11] | 6.10[15] | 1.50[−11] |
| $Ta^{45+}$ | 887 | 4.09[15] | 2.51[15] | 2.14[16] | 1.32[16] | 2.85[−11] | 8.60[15] | 1.78[−11] |
| $Au^{51+}$ | 1044 | 6.37[15] | 2.68[15] | 2.27[16] | 1.60[16] | 2.95[−11] | 1.06[16] | 1.87[−11] |
| $At^{57+}$ | 1211 | 9.47[15] | 2.79[15] | 2.36[16] | 1.83[16] | 2.84[−11] | 1.28[16] | 1.89[−11] |
| $U^{64+}$ | 1421 | 1.42[16] | 2.93[15] | 2.48[16] | 2.06[16] | 2.61[−11] | 1.51[16] | 1.81[−11] |

eling a dense laser-produced plasma. The previous sections led to the conclusion that for the $3d^94l4l'$ complex, detailed *level-by-level* computations including configuration mixing, nonresonant decays, and in some cases cascades, are necessary when accurate results for the rates of DR through this complex are sought. One might suggest that averaging methods are adequate at least for the $3d^94l5l'$ complex, even in the case of plasmas which are not so dense, and where the level depleting collisions are negligible. Thus the use of average quantities for the evaluation of the DR rate coefficients along the isoelectronic sequence has been tested here for the particular $3d^94f5f$ configuration. For these test calculations the NRS and DAC processes have been neglected for simplification, and also in order to enable comparison of the present results to those of Ref. [12], where this approximation was used. Including only resonant radiative decays, the mean DR rate coefficient for a given configuration $c$ is defined by

$$\overline{\alpha_c^D} = 1.656\times 10^{-22} kT_e^{-3/2} \times \exp\left(\frac{-\overline{\Delta E_c}}{kT_e}\right) \frac{1}{g_k} \frac{\left(\sum_d g_d A_{dk}^a\right)\left(\sum_d \sum_i A_{di}\right)}{\sum_d \sum_{k'} A_{dk'}^a + \sum_d \sum_i A_{di}}, \tag{7}$$

where $\overline{\Delta E_c} = \overline{E_c} - E_I$, $\overline{E_c}$ being the statistically weighted average energy of the configuration and $E_I$ the ionization energy. $\overline{\Delta E_c}$ and $kT_e$ are expressed in eV. Here, $\Sigma\Sigma A_{di}$ represents the sum of the radiative decay coefficients for all the transitions $3d^94f5f \rightarrow 3d^{10}n''f$ $(n''=4,5)$, $\Sigma\Sigma A_{dk'}^a$ is the sum of the coefficients for autoionization to all possible Ni-like states, and $\Sigma g_d A_{dk}^a$ is the statistically weighted sum of the coefficients for autoionization to $3d^{10}$.

Table IV displays in the second through sixth columns the computed quantities involved in Eq. (7) for the $3d^94f5f$ configuration for the ten ions considered. These quantities for $Ta^{45+}$ have been previously calculated by Bauche-Arnoult *et al.* [12], and are in good agreement with the present results. In Ref. [12] the quantity $\Sigma\Sigma g_d A_{di}$ was calculated instead of $\Sigma\Sigma A_{di}$ and a value of $2.66\times 10^{16}$ s$^{-1}$ was obtained, compared to $2.86\times 10^{16}$ s$^{-1}$ for the same quantity using the present computation method. For $\Sigma g_d A_{dk}^a$ the values calculated in Ref. [12] and in the present work are $2.07\times 10^{16}$ and $2.14\times 10^{16}$ s$^{-1}$, respectively.

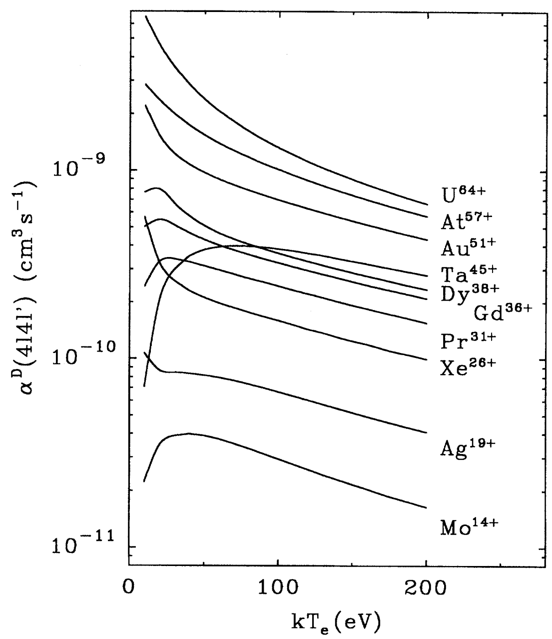


FIG. 2. Rate coefficients for DR of Ni-like ions through the whole Cu-like $3d^94l4l'$ complex as a function of the electron temperature.

The $\overline{\alpha_c^D}$ coefficients calculated at $kT_e = 1$ keV are listed in the seventh column. In order to evaluate the accuracy of these results, the DR rate coefficients $\alpha_c^D$ obtained by detailed level-by-level computations at the same electron temperature are given in the ninth column for comparison. The results of the sum term $\Sigma(gA^a\Sigma A/\Sigma A^a + \Sigma A)$ involved in the exact calculation of $\alpha_c^D$ [Eqs. (4′), (5), and (6)] are given in the eighth column.

The discrepancy between the two coefficients $\overline{\alpha_c^D}$ and $\alpha_c^D$ varies from a factor of 1.75 for $Ag^{19+}$ to a factor of 1.44 for $U^{64+}$. In all these cases $\overline{\alpha_c^D}$ gives an overestimated value.

TABLE V. Rate coefficients (in cm$^3$ s$^{-1}$) for DR of Ni-like ions through the whole Cu-like $3d^94l4l'$ configuration complex at different electron temperatures. $X[-Y]$ denotes $X\times 10^{-Y}$.

| | $T_e$ | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Ion | 10 eV | 20 eV | 50 eV | 100 eV | 200 eV | 500 eV | 1000 eV | 2000 eV | 5000 eV | 10 000 eV |
| $Mo^{14+}$ | 2.23[−11] | 3.48[−11] | 3.90[−11] | 2.94[−11] | 1.64[−11] | 5.63[−12] | 2.21[−12] | 8.25[−13] | 2.16[−13] | 7.71[−14] |
| $Ag^{19+}$ | 1.07[−10] | 8.67[−11] | 8.16[−11] | 6.65[−11] | 4.08[−11] | 1.51[−11] | 6.11[−12] | 2.31[−12] | 6.10[−13] | 2.19[−13] |
| $Xe^{26+}$ | 5.65[−10] | 3.23[−10] | 2.11[−10] | 1.59[−10] | 9.94[−11] | 3.84[−11] | 1.58[−11] | 6.07[−12] | 1.61[−12] | 5.79[−13] |
| $Pr^{31+}$ | 2.43[−10] | 3.29[−10] | 3.11[−10] | 2.43[−10] | 1.55[−10] | 6.12[−11] | 2.55[−11] | 9.82[−12] | 2.62[−12] | 9.41[−13] |
| $Gd^{36+}$ | 5.05[−10] | 5.49[−10] | 4.29[−10] | 3.23[−10] | 2.09[−10] | 8.44[−11] | 3.55[−11] | 1.37[−11] | 3.67[−12] | 1.32[−12] |
| $Dy^{38+}$ | 7.68[−10] | 7.94[−10] | 5.09[−10] | 3.63[−10] | 2.33[−10] | 9.45[−11] | 3.98[−11] | 1.54[−11] | 4.13[−12] | 1.49[−12] |
| $Ta^{45+}$ | 7.11[−11] | 2.06[−10] | 3.80[−10] | 3.83[−10] | 2.78[−10] | 1.18[−10] | 5.04[−11] | 1.96[−11] | 5.27[−12] | 1.90[−12] |
| $Au^{51+}$ | 2.21[−9] | 1.52[−9] | 9.70[−10] | 6.97[−10] | 4.32[−10] | 1.69[−10] | 7.02[−11] | 2.70[−11] | 7.19[−12] | 2.59[−12] |
| $At^{57+}$ | 2.86[−9] | 2.35[−9] | 1.54[−9] | 1.01[−9] | 5.73[−10] | 2.10[−10] | 8.54[−11] | 3.25[−11] | 8.60[−12] | 3.09[−12] |
| $U^{64+}$ | 6.54[−9] | 4.58[−9] | 2.39[−9] | 1.32[−9] | 6.67[−10] | 2.27[−10] | 9.03[−11] | 3.40[−11] | 8.92[−12] | 3.20[−12] |

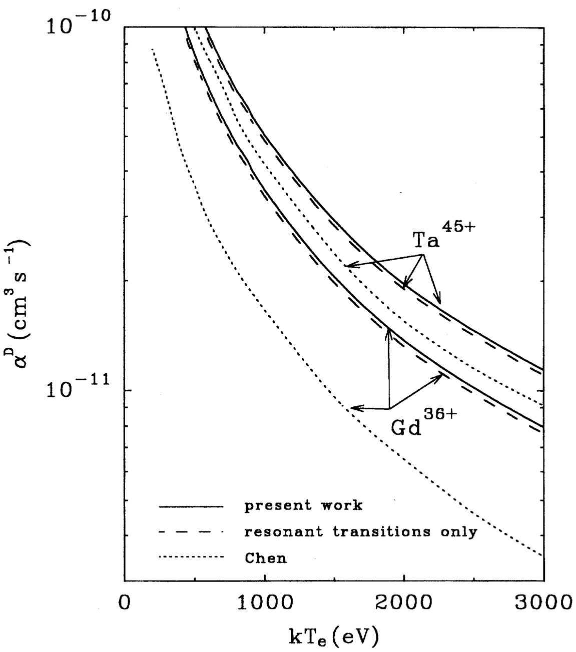


FIG. 3. Rate coefficients for DR of $Gd^{36+}$ and $Ta^{45+}$ through the $3d^94l4l'$ configuration complex as a function of the electron temperature. Solid lines show the present results including nonresonant transitions and cascades, and dashed lines the results taking into account the resonant transitions only. Dotted lines represent the results of Refs. [6,7].

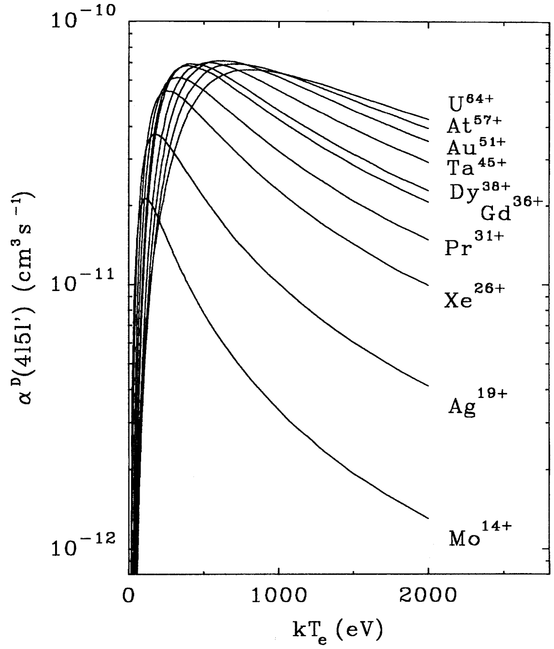


FIG. 4. Rate coefficients for DR of Ni-like ions through the whole Cu-like $3d^94l5l'$ complex as a function of the electron temperature.

The deviation of $\overline{\alpha_c^D}$ along the sequence cannot result from the inaccuracy of the mean energy approximation, since the exponent term in Eq. (7) varies relatively slowly from level to level within the configuration $c$ in the considered $0.2<\overline{\Delta E_c}/kT_e<1.5$ range. The discrepancies should instead be attributed to the poor correlation between the autoionization and the radiative decay coefficients for individual levels. This is evident by comparing the values of the sum term in the sixth column appearing in the $\overline{\alpha_c^D}$ expression [Eq. (7)] to those of the sum term in the eighth column involved in the exact calculation of $\alpha_c^D$. The ratio of these two terms (which varies from 1.72 for Ag to 1.36 for U) is extremely close to the ratio of $\overline{\alpha_c^D}$ to $\alpha_c^D$ (from 1.75 to 1.44). Hence, clearly the discrepancy between $\overline{\alpha_c^D}$ and $\alpha_c^D$ is mostly due to the discrepancy between the two sum terms.

In the case of $Mo^{14+}$ the $\overline{\alpha_c^D}$ calculations show that this discrepancy disappears; this is correlated to the possible autoionization to excited $3d^94l$ levels, which is almost negligible for $Ag^{19+}$ and becomes totally impossible for the heavier ions of the sequence. This process has been included in the $\Sigma A_{dk'}^a$ sums in both $\alpha_c^D$ and $\overline{\alpha_c^D}$ calculations for the low-$Z$ elements. The autoionization to $3d^94l$ levels increases the correlation between autoionization and radiative decay for almost all levels.

The same kind of calculations were also carried out for the $3d^94f^2$ configuration, and the mean coefficient $\overline{\alpha_c^D}$ was similarly found to overestimate the DR rate coefficients along the sequence, in this case by a factor of 2.22 (for Mo) to 1.74 (for U). The results for these two particular configurations can give an idea of the accuracy limitation expected from the configuration averaging method in general. It should be added that for DR through higher lying configurations the effect of autoionization to Ni-like excited levels is expected to increase. For these configurations the accuracy of the average method evaluation is also unpredictable.

It should be stressed that in dense plasmas (as considered in Ref. [12]) the populations of the high-$n$ levels within the inner-shell excited configurations may become statistically redistributed by collisions, and even the low-$n$ states in high-$Z$ ions might undergo a partial redistribution. In these conditions the mean DR rate coefficients $\overline{\alpha_c^D}$ may be expected to reflect the actual DR rates better than in the present model where level depleting collisions are negligible. In such dense plasmas the validity of the average rate approximation should be checked by comparison to a precise modeling based on the collisional-radiative approach [15].

## IV. RESULTS

In the following sections the final results of the computations performed using detailed level-by-level calculations, including NRS and DAC processes, for the ten considered elements along the Ni I isoelectronic sequence are presented.

### A. DR through the $3d^94l4l'$ complex

Figure 2 displays the total rate coefficients for DR through the whole $3d^94l4l'$ configuration complex as a function of the electron temperature in the 10 eV $\leq kT_e \leq 200$ eV range for the ten ions considered. The fact that some levels of the $3d^94l4l'$ configurations may be above the ionization limit and very close to it for some ele-

TABLE VI. Rate coefficients (in $cm^3\ s^{-1}$) for DR of Ni-like ions through the whole Cu-like $3d^9 4l5l'$ configuration complex at different electron temperatures. $X[-Y]$ denotes $X \times 10^{-Y}$.

| | $T_e$ | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|
| Ion | 10 eV | 20 eV | 50 eV | 100 eV | 200 eV | 500 eV | 1000 eV | 2000 eV | 5000 eV | 10 000 eV |
| $Mo^{14+}$ | 2.79[−13] | 2.42[−12] | 1.31[−11] | 2.11[−11] | 1.77[−11] | 7.80[−12] | 3.35[−12] | 1.30[−12] | 3.48[−13] | 1.26[−13] |
| $Ag^{19+}$ | 2.52[−14] | 7.61[−13] | 1.05[−11] | 2.93[−11] | 3.70[−11] | 2.15[−11] | 1.01[−11] | 4.12[−12] | 1.13[−12] | 4.13[−13] |
| $Xe^{26+}$ | 1.18[−15] | 1.25[−13] | 5.44[−12] | 2.60[−11] | 5.19[−11] | 4.25[−11] | 2.28[−11] | 9.94[−12] | 2.85[−12] | 1.05[−12] |
| $Pr^{31+}$ | 2.32[−16] | 4.05[−14] | 2.83[−12] | 1.89[−11] | 5.10[−11] | 5.48[−11] | 3.22[−11] | 1.48[−11] | 4.37[−12] | 1.63[−12] |
| $Gd^{36+}$ | 7.69[−17] | 1.72[−14] | 1.49[−12] | 1.29[−11] | 4.69[−11] | 6.80[−11] | 4.61[−11] | 2.28[−11] | 7.07[−12] | 2.67[−12] |
| $Dy^{38+}$ | 6.00[−17] | 1.37[−14] | 1.17[−12] | 1.10[−11] | 4.40[−11] | 5.27[−11] | 3.74[−11] | 1.88[−11] | 7.91[−12] | 2.23[−12] |
| $Ta^{45+}$ | 1.03[−16] | 1.36[−14] | 6.25[−13] | 6.32[−12] | 3.20[−11] | 7.09[−11] | 5.59[−11] | 2.99[−11] | 9.68[−12] | 3.72[−12] |
| $Au^{51+}$ | 1.41[−15] | 4.35[−14] | 5.48[−13] | 4.58[−12] | 2.39[−11] | 6.88[−11] | 6.17[−11] | 3.52[−11] | 1.20[−11] | 4.67[−12] |
| $At^{57+}$ | 4.65[−13] | 7.17[−13] | 9.16[−13] | 4.23[−12] | 1.87[−11] | 6.33[−11] | 6.41[−11] | 3.94[−11] | 1.40[−11] | 5.54[−12] |
| $U^{64+}$ | 1.49[−14] | 1.35[−13] | 1.27[−12] | 5.45[−12] | 1.70[−11] | 5.55[−11] | 6.39[−11] | 4.27[−11] | 1.59[−11] | 6.43[−12] |

ments can lead to a complex behavior of the DR rate coefficients as a function of the electron temperature, as can be seen in Fig. 2. In the temperature range exhibited, DR through $3d^9 4l4l'$ (for which the $\Delta E_d$ values are low) is the prevalent DR process especially for heavy elements due to the exponential dependence on $-\Delta E_d / kT_e$ [Eq. (3)]. As can be seen in Fig. 2, at low electron temperature the DR coefficients show a rather complex dependence on $T_e$, which differs from ion to ion. This is explained by the fact that some autoionizing levels very close to the ionization limit can considerably enhance the DR rate. Indeed, one can show from Eq. (3) that the contribution of a given level $d$ to the DR rate as a function of $T_e$ reaches a maximum value at $kT_e = 2/3 \Delta E_d$. This maximum value is proportional to $(\Delta E_d)^{-3/2}$. Consequently, if $\Delta E_d$ is sufficiently small the contribution of this level at low $T_e$ might be very important. For instance, our theoretical calculations predict that one of the $3d^9 4p4d$ levels of $Xe^{25+}$ lies less than 1 eV above the ionization limit, and for this reason will give a dominant contribution to the total DR rate at low temperature ($kT_e < 10$ eV). This is reflected in Fig. 2 by the remarkably steep ascent of the $Xe^{26+}$ curve as the temperature decreases. The contribution of this level is still not negligible at 100 eV. However, it must be stressed that in such cases the accuracy of the theoretical predictions can be questioned, since the magnitude of the DR coefficient depends on the very small difference between the computed values for the energy of the level and the ionization limit, both having an accuracy of the order of 0.1%. Moreover, a small error in the computed energy of levels so close to the ionization limit could lead to an erroneous prediction of the opening (or closing) of a very strong DR channel. In conclusion, the change in the position of levels from above to below the ionization limit along the isoelectronic sequence causes the variation in the $T_e$ dependence of the DR rate coefficients observed in Fig. 2. For some ions very high values are observed at low electron temperature.

In these cases in particular, the DR rate coefficients cannot be accurately evaluated by the semiempirical Burgess-Merts approximation [8,9]. The major simplification made in this approximation was to assume that the main contribution to DR comes from levels with very high values of $n'$ and $l'$. This assumption, which may be sufficiently accurate for weakly ionized ions pertaining to sequences isoelectronic to light elements, is obviously no longer valid for DR through the Cu-like $3d^9 4l4l'$ complex.

Table V gives the computed rate coefficients for DR through the whole $3d^9 4l4l'$ complex at different electron temperatures in the 10 eV–10 keV range. In these calculations the full effects of configuration mixing, NRS, and DAC were included. Figure 3 shows the present DR results for $3d^9 4l4l'$ in the case of $Gd^{36+}$ and $Ta^{45+}$ compared to those obtained by Chen using the multiconfiguration Dirac-Fock method (Ref. [6], Fig. 1 therein and Ref. [7], Fig. 2). Only the resonant radiative transitions were included in those two works. The Ta results are in quite good agreement (between 10% and 15%) with the present results. For Gd, however, the

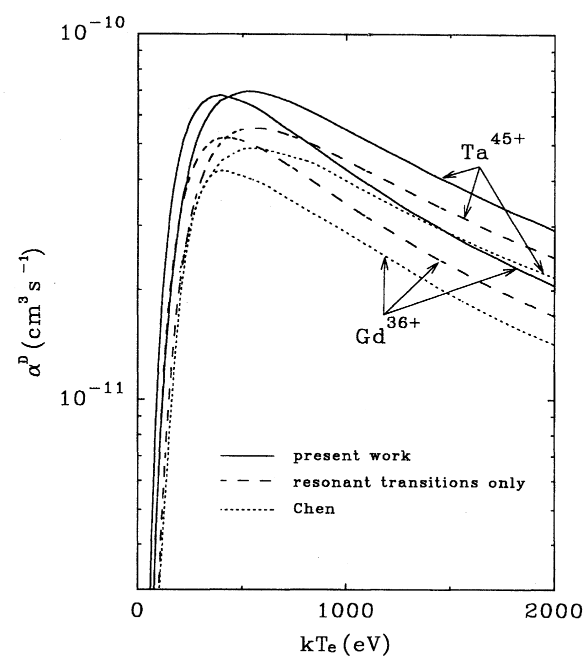


FIG. 5. Rate coefficients for DR of $Gd^{36+}$ and $Ta^{45+}$ through the $3d^9 4l5l'$ configuration complex as a function of the electron temperature. Solid lines show the present results including nonresonant transitions and cascades, and dashed lines the results taking into account the resonant transitions only. Dotted lines represent the results of Refs. [6,7].

discrepancy is of a factor of about 2. In both these cases the present results are higher, and the discrepancies increase only very little when including NRS and DAC (Fig. 3).

### B. DR through the $3d^9 4l5l'$ complex

Figure 4 shows the total rate coefficients for DR through the whole $3d^9 4l5l'$ configuration complex as a function of the electron temperature in the 10 eV$\leq kT_e \leq$200 eV range for the ten ions considered. In this complex all the 2011 levels lie above the ionization limit for all the elements. For this reason, as can be seen in Fig. 4, the dependence of the DR rate coefficients on the electron temperature is quite regular even at low temperature, in contrast to the previous $3d^9 4l4l'$ case (Fig. 2). For relatively low-$Z$ elements (Mo to Ag) autoionization to Ni-like excited configurations (mainly $3d^9 4s$ and $3d^9 4p$) is possible, and has been taken into account in the present computations. It was found that this process reduces the rates of DR through the whole $3d^9 4l5l'$ complex by only a few percent.

Table VI shows the results of the detailed level-by-level computations of the rate coefficients for DR through the $3d^9 4l5l'$ complex for the ten Ni-like ions considered. In these calculations the effect of the NRS and DAC decays to the $3d^9 4l4l'$ complex has been included. The relatively high rates for At and U at low electron temperature are a direct result of the remarkably strong NRS effect discussed in the preceding section. Since for the $3d^9 4l5l'$ complex the effect of configuration interactions is much less critical (Sec. III B), they have been neglected.

For this complex, the discrepancy between our results and those obtained in Refs. [6,7] is between 20% and 40% for both Gd and Ta, as can be seen in Fig. 5. Including only resonant transitions as in Refs. [6,7] the discrepancy is cut down to a relative value of 10–20 %.

## V. CONCLUSION

Detailed level-by-level calculations of the rate coefficients for DR of ground state Ni-like ions through the Cu-like inner-shell excited configuration complexes $3d^9 4l4l'$ and $3d^9 4l5l'$ have been performed. The results are presented for ten ions of the isoelectronic sequence. It is shown that nonresonant stabilizing radiative transitions can produce a significant enhancement of the DR through both complexes especially at low temperature, and thus must be taken into account. The effect of decays to autoionizing levels followed by cascades is much smaller, of the order of a few percent or even less. The results show that the $3d^9 4l4l'$ complex gives the main contribution to DR at low temperature due to the fact that the excited levels of this complex lie close to the ionization limit. In this case, only detailed calculations including configuration mixing are reliable since the number of levels participating in the DR process varies from ion to ion. Even for the $3d^9 4l5l'$ configuration complex, in which all the levels are above the ionization limit and configuration interactions are relatively unimportant, one should still take with caution the results of average models which can lead to an overestimation of the DR rates by a factor of up to 2.

## ACKNOWLEDGMENTS

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