

§11. Quantum-Mechanical Interference in Photorecombination of Sc^{3+}

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Most of atomic data of photorecombination processes used in plasmas is based on independent calculations for radiative and dielectronic recombination (RR and DR). DR-RR interference is not considered in general. Especially, it is taken for granted to omit the interference effects in recombination for low- or medium-Z ions. Recently Gorczyca *et al*¹ predicted a unusually large DR-RR interference effect in recombination of Sc^{3+} theoretically. However, the experimental search for the strong DR-RR interference effect failed² (see Fig. 1), and the comparison displays the several peaks observed are not given by Gorczyca *et al*.

We have carried out both nonperturbative and perturbative calculations for the $e + Sc^{3+}$ photorecombination. The nonperturbative method is based on the rigorous continuum-bound transition theory and the close-coupling R-matrix approach. The perturbative evaluation is a treatment including DR, RR, and their interference. The rate coefficients are presented in Fig. 2. Our calculations showed that the appearance of the several experimental resonance peaks, which were not predicted by Gorczyca *et al* in the LS-coupling scheme, is attributed to relativistic effects. For example, the LS coupling calculations do not give the resonance $3p^5 3d^2 [^3F] ^2D^o$ at about 16.9 eV due to limitation of the angular momentum and parity conservation. Only when spin-orbit interaction is taken into account, can corresponding recombination happen. It should be pointed out that in general, the resonances that stem from the relativistic effect are of small Auger widths if the atomic number Z is not large. However, a very narrow resonance may play an important role in recombination. This is because whether a resonance is significant depends not only on Auger and radiative widths of the resonances themselves but also on the Auger and radiative widths of the dominant resonances. Therefore, it is unsafe to omit relativistic effects for recombination of low- or medium-Z ions with no check.

We noticed that the interference effect between the resonance $3p^5 3d^2 [^3F] ^2F$ and the background, predicted by Gorczyca *et al*¹, is reproduced by our calculation in the LS coupling scheme. But when relativistic effects are considered, the two new peaks on the left side of the $3p^5 3d^2 [^3F] ^2F$ appear, as shown in the experiment. Thus the interference effect is masked on the left side of the resonance by the adjacent resonances. On the other side of the resonance, the results calculated are much higher than the experiment. We calculated RR, DR, and interference cross sections in perturbation theory, and found

that just the RR should be responsible for the great discrepancy. A possible reason is that the RR cross section is greatly overestimated because of the difficulty to describe the many-electron systems exactly. We tried to employ the 1/10 times the RR cross sections to evaluate the interference and total cross sections including DR, RR and interference terms. A very good agreement with the experiment has been shown (here the result is not given). Even so, further experimental and theoretical studies are required. For example, considering the high resolution in photoionization experiments, we call for an observation of photoionization of Sc^{2+} in the $3p^6 3d ^2D$ state to examine the recombination measurement and calculations.

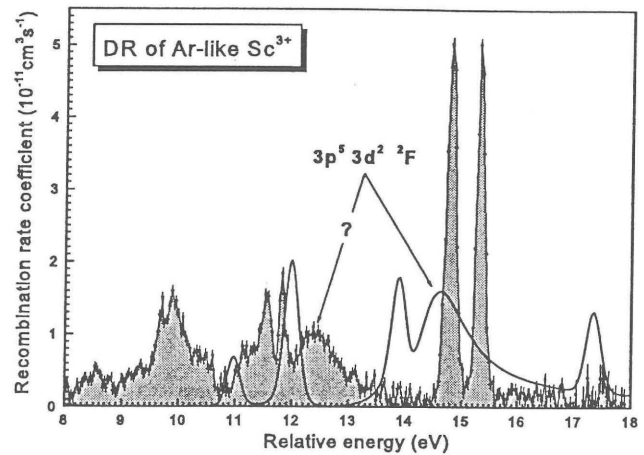


Fig. 1 The measured rate coefficients for Sc^{3+} compared with the calculation of Gorczyca *et al*¹ (full line).

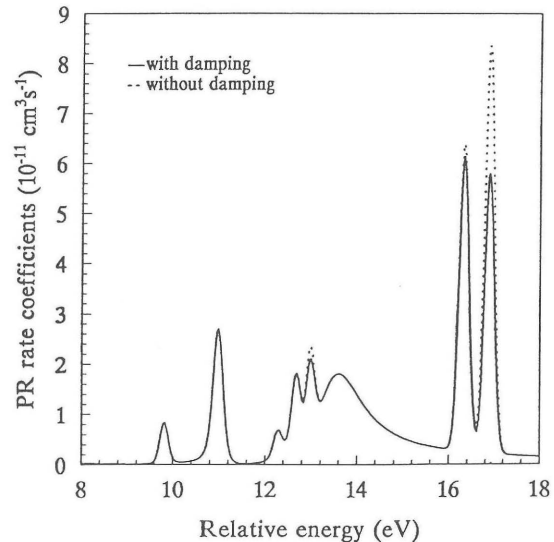


Fig. 2 The calculated rate coefficients for Sc^{3+}

Reference

- 1) T. W. Gorczyca *et al*, Phys. Rev. A **56**, 4742 (1997).
- 2) S. Schippers *et al*, Phys. Rev. A. (to be submitted)