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Ionization and Recombination in Transition Metal Ions

N. R. Badnell and M. S. Pindzola

Department of Physics, Auburn University, Auburn, Alabama, 36849-5311, USA

D. C. Griffin

Department of Physics, Rollins Collge, Winter Park, Florida 32789, USA

and

H. P. Summers

JET Joint Undertaking, Abingdon, Oxon, OX14 3EA, UK

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Abstract

We discuss atomic data for transition metal ions and its use in the modeling of non-LTE magnetic fusion plasmas.

Atomic data is required for transiton metal ions both for diagnostic purposes [1], and for the modeling of magnetic fusion edge-plasmas [2]. Data is always available from simple semi-empirical formulae but this is often subject to large errors. Consequently, data-bases [3] are continually being updated with the results of detailed quantum mechanical calculations. The accuracy of this data is assessed by detailed comparisons with experimental measurements for isolated ions (i.e., zero-density). The zero-density data is then incorporated [3] into the solution of the collisional dielectronic population rate equations [4] from which level populations [5], ionization balance [6] and power loss [7] can be determined for a finite-density plasma.

The theoretical data for ionization is quite substantial. Rate coefficients, including excitation-autoionization, have been calculated for the ground and metastable states for the complete Fe [8] and Ni [9] insonuclear sequences. Calculations have also been carried out for a number of Ti [10] ions from which the accuracy of the extrapolation of the Fe and Ni data to other ions can be assessed. Comparisons have also been made with the results of a number of experiments which indicate a typical accuracy of 25% for the total ionization rate coefficient. Some illustrative results are shown in Fig. 1. Further details pertaining to the ionization data may be found in an accompanying paper in this special issue.

The data for recombination, which is usually dominated by dielectronic recombination, is less substantial. The calculation of dielectronic recombination rate coefficients for the complete Fe isonuclear sequence is in progress for all the dominant transitions in a combination of configuation-average, *LS*-coupling and intermediate coupling schemes. Results for Fe^{q+} (q = 15, 21–25) have already been calculated [11] and some illustrative (zero-density) results are shown in Fig. 2. This data can be incorporated [3] into the solution of the collisional dielectronic population rate equations [4] for a finite-density plasma by parameterizing raw data calculated with the Burgess General Program [3] in the bundled-*nl* or bundled-*n* pictures [3, 5]. In many cases, this ordinary picture [4] must be modified to take account of

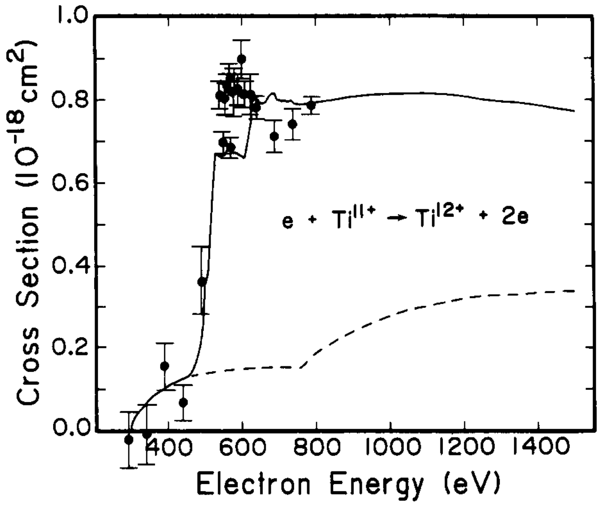

Fig. 1. Comparison of theory and experiment for the ionization of Ti^{11+}, taken from Chantrenne *et al.* (see Ref. [10]).

metastables [7, 5, 2]. In the generalised picture [7] we require as input rate coefficients from the ground and metastables as well as cross terms from the metastables back to the ground. This data can then be incorporated into the solution of the generalized collisional dielectronic rate equations. This has already been done for the C and O isonuclear sequencies [12] which were the subject of the last IAEA specialists meeting [13]. Some illustrative generalized collisional dielectronic

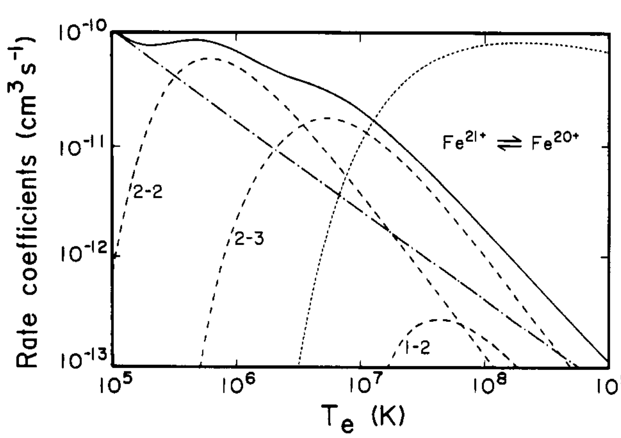

Fig. 2. Ionization and recombination rate coefficients for $Fe^{20+} \rightleftharpoons Fe^{21+}$ taken from Badnell (see Ref. [11]).

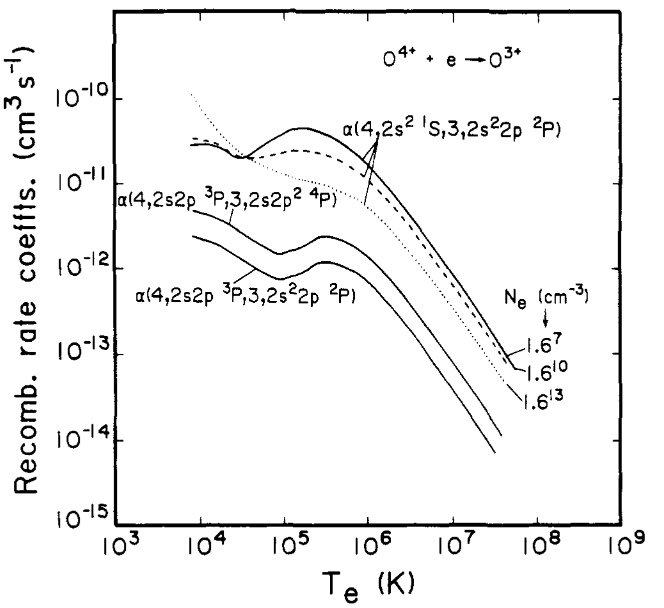

Fig. 3. Generalized collisional dielectronic recombination rate coefficients for O^{4+} to O^{3+}.

recombination rate coefficients are given in figure 3 for O^{4+}. Here, the ground-to-ground coefficient is $2s^2\ ^1s \rightarrow 2s^2 2p\ ^2P$, the metastable-to-metastable is $2s2p\ ^3P \rightarrow 2s2p^2\ ^4P$ and the metastable-to-ground is $2s2p\ ^3P \rightarrow 2s^2 2p\ ^2P$.

Since dielectronic recombination is so sensitive to density effects, it would be useful to have an a priori estimate of the collision limit from which a rough effective dielectronic recombination rate coefficient could be estimated from zero-density data without the solution of the population rate equations. The Wilson [14] formula does not fulfil this requirement. It was derived before the importance of dielectronic recombination was recognized and so grossly underestimates the collision limit. Consequently, calculations [15] of density-dependent dielectronic recombination rate coefficients based on the Wilson formula should be treated with caution. We close by noting that the effect of electric fields on dielectronic recombination, which is substantial in a merged-beam experiment, is likely to be dominated by collision effects in a magnetic fusion plasma; just compare the continuum lowering due to the plasma microfield [16] with that due to electron collisions [4].

Note added in proof

A bibliography of zero-density dielectronic recombination data for transition metal ions is contained in the contribution from Hahn in this special issue.

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