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Electron-impact ionization of Fe^{3+}

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Synopsis Electron-impact ionization cross sections are studied for levels of the ground and first excited configurations of the Fe^{3+} ion. Convergence for the excitation-autoionization cross sections due to excitations to the high-nl shells is investigated. Single configuration and configuration interaction methods are used in the study. Scaling is applied to the distorted wave cross sections of the excitation-autoionization and collisional ionization processes.

Fundamental atomic data of ionization and recombination processes are necessary for identification of the composition of astrophysical plasmas, modeling the structure and dynamics of laboratory plasma and high-temperature plasmas in stars.

In this work, electron-impact ionization for the Fe^{3+} ion is investigated. The study of direct ionization (DI) and excitation-autoionization (EA) processes is carried out for levels of the ground [Ne]$3s^2 3p^6 3d^5$ and first excited [Ne]$3s^2 3p^6 3d^4 4s$ configurations. Convergence for the EA cross sections due to excitations to the high-nl shells is investigated.

Energy levels, radiative and Auger transition probabilities, electron-impact excitation and ionization cross sections for the Fe^{3+} ion are generated using the Flexible atomic code (FAC) [1]. The code implements the Dirac-Fock-Slater approach. Electron-impact ionization and excitation cross sections are obtained in the distorted wave (DW) approximation. Single configuration and configuration interaction (CI) methods are used in the study of ionization cross sections. In addition, scaling is applied to the DW cross sections of the EA and DI processes.

Previous calculations for the ionization cross sections of Fe^{3+} were performed using the configuration-average DW approach [2]. Our data shows that many configurations have energy levels that straddle the single ionization threshold. This demonstrates that study of energy levels is needed.

Comparison of theoretical cross sections with experimental values for Fe^{3+} is presented in Fig. 1. Theoretical data correspond to the $3d^2_{3/2}(2)3d^2_{5/2}(4)4s_{1/2}$ $J = 13/2$ level. It can be seen that scaling plays an important role in producing a better agreement with measurements. However, the scaled single-configuration results overestimate the experimental values at the lower energies of the incident electron. On the other hand, the scaled CI data are below the measurements near the peak of cross sections on the low energy side. The good agreement with experimental values is obtained at the higher energies for both scaled calculations.

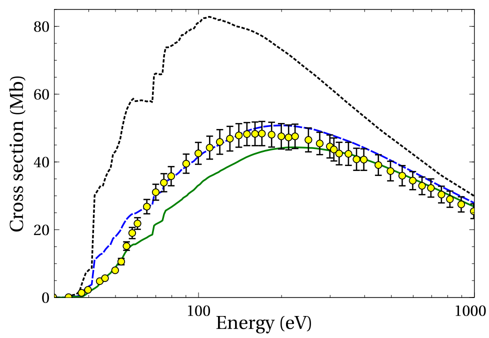

Figure 1. Comparison of theoretical cross sections with experimental values [3]. Dotted line (black) - single-configuration, dashed line (blue) - scaled single-configuration, and solid line (green) - scaled CI calculations.

References

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