Distorted wave photoionization cross sections for use in NLTE model atmospheres: Ni – Ni^{10+}

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Synopsis The Opacity Project is a highly successful venture in which energy levels, oscillator strengths, and photoionization cross sections were calculated for astrophysically important elements up to iron. However, metals heavier than iron are being discovered in stellar atmospheres. The photoionization cross sections for elements and ions not covered by the Opacity Project are usually approximated with hydrogenic formulae. We present a series of valence and inner-shell distorted wave photoionization cross section calculations for use in model atmosphere calculations covering Ni^{00+} - Ni^{10+}. We discuss current progress, and future work.

Stellar atmosphere models can only ever be as good as the atomic data supplied to them. The Opacity Project has served as a gold standard for atomic data for use in opacity calculations and bespoke stellar atmosphere modelling. The Opacity Project has calculated energy levels, oscillator strengths, and photoionization cross sections for all astrophysically relevant ions up to iron. Beyond iron, the photoionisation cross sections are usually approximated with hydrogenic formulae, or extrapolated. There do exist distorted wave calculations by [1], however, these are totals only and are not partially resolved. In the case of white dwarf stars, hydrogenic cross sections are a poor approximation. [2] considered the effect on measured atmospheric abundances for the hot white dwarf G191-B2B when using model atmospheres calculated with hydrogenic and realistic nickel PI data. It was shown that the abundances and the flux distribution in the extreme ultraviolet wavelengths changed dramatically, with flux attenuation being 80% greater in the realistic case compared to the hydrogenic case. This result alone is motivation to continue the work of the Opacity Project and calculate PI data for heavier metals. To this end, we present our progress in calculating valence and inner-shell PI data for Ni^{00+} - Ni^{10+}.

The cross sections were calculated using the distorted wave code AUTOSTRUCTURE [3] We treat PI from different complexes separately, splitting the calculation into K-shell, L-shell, and M-shell respectively. This is a valid approximation to make, as mixing between levels arising from K, L, and M-Shell PI is small. The K and L-Shell cross sections were calculated with term resolution, and the M-Shell cross sections were calculated with level resolution using kappa-averaged relativistic wavefunctions. An example of the data calculated is given in Figure 1, where we have plotted the total direct PI cross sections for Ni10+, while also showing the individual contributions from the K, L, and M shells.

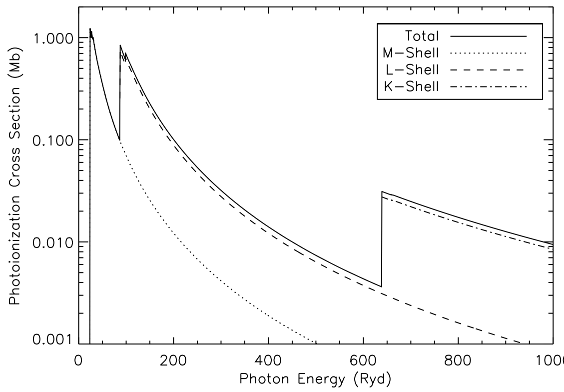

Figure 1. Total direct photoionization cross section of Ni^{10+} (solid line), along with contributions from M-Shell (dotted line), L-Shell (dashed line), and K-Shell (dot dashed line) photoionization.

Currently, direct PI cross sections have been calculated for Ni^{00+}-Ni^{10+}. We intend to calculate the resonant contributions to the total PI cross section. In addition, we will assess the effect of this atomic data on white dwarf model atmospheres, and in particular, changes to atmospheric structure, temperature, and atmospheric abundances.

References

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