Benchmark calculations for electron collisions with neutral indium atoms

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Introduction

Motivation:

- Indium (In) is currently used to make transparent electrodes in liquid-crystal displays (LCDs) [1].
- It is a candidate to replace mercury in low-pressure discharge lamps [1].
- Its spectral lines are expected to be very important in modeling plasmas in which indium is a constituent.
- It is particularly suitable as a tracer for two-line atomic fluorescence (TLAF) thermometry measurements [2].
- Despite its various applications, there currently is a lack of electron-indium scattering data available.

Goal: Provide a set of accurate cross-section data, over a wide energy range, for use in gas-discharge and low-temperature plasma modeling.

Methods

B-Spline R-Matrix (BSR):

- Variant of the R-matrix method to solve the close-coupling equations in coordinate space [3].
- B-spline basis for the radial functions.
- Uses non-orthogonal bound and continuum orbitals - high level of accuracy with compact configuration expansions.

Convergent Close Coupling (CCC):

- Uses an integral equation formulation of the close-coupling equations in momentum-space [4].
- Complete square-integrable basis with convergence being obtained by increasing the basis size.
- Can currently handle quasi one- and two-electron systems.

Results

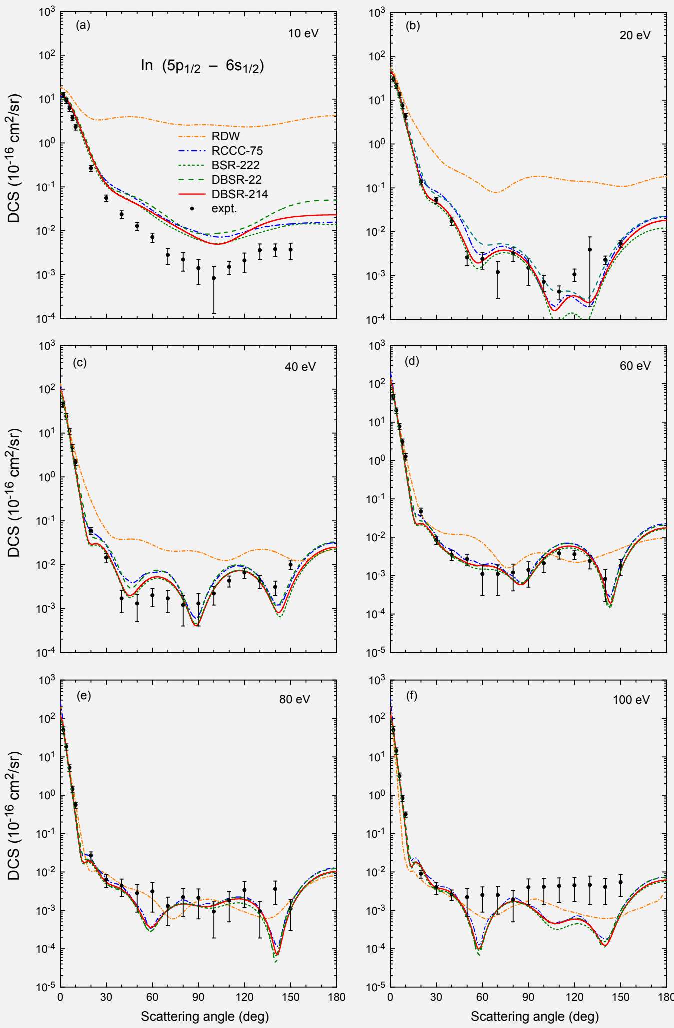


Fig.1: Angle-differential cross section for electron-impact excitation of the $(5s^2 5p)^2P^o_{1/2} \rightarrow (5s^2 6s)^2S_{1/2}$ transition in neutral indium at various incident projectile energies. Results from (D)BSR and RCCC calculations are compared with Relativistic Distorted Wave (RDW) predictions and experimental results [5]. DBSR and RCCC-N indicate that N states were included in the close-coupling expansion.

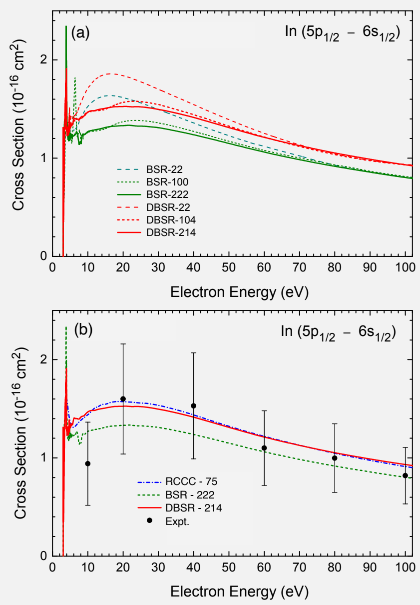


Fig.2: Angle-integrated cross section for electron-impact excitation of the $(5s^2 5p)^2P^o_{1/2} \rightarrow (5s^2 6s)^2S_{1/2}$ transition in neutral indium. Resulting cross sections from different sizes of (D)BSR models are shown in (a), and DBSR, BSR and RCCC results are compared with experimental data in (b).

Lower State	Upper state	NIST	DBSR (L)	DBSR (V)
$(5s^2 5p)^2P^o_{1/2}$	$(5s^2 6s)^2S_{1/2}$	0.14	0.135	0.129
$(5s^2 5p)^2P^o_{1/2}$	$(5s^2 5d)^2D_{3/2}$	0.36	0.349	0.341

Table 1: Oscillator strengths of two different transitions in indium obtained from the DBSR model. L and V indicate the results obtained with the length and velocity form of the dipole operator, respectively.

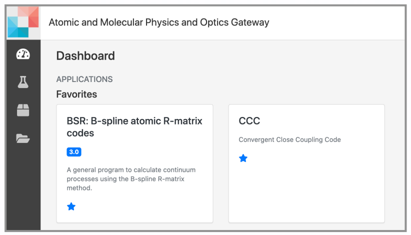
BSR Indium ground-state polarizability: $64.5\ a_0^3$

Experiment: $56.1 \pm 18.2\ a_0^3$ [6]

Conclusion

- Generally excellent agreement was found between the highest-level RCCC-75 and DBSR-214 calculations, in both the DCS and ICS.
- Very good agreement was found between those calculations and experimental data, with the main exception of 10 eV and for scattered electron angles >10°.
- We believe a recommended 6s data set could be formed by taking an average, at any energy, between our RCCC-75 and DBSR-214 calculations (uncertainty ±10%).
- Structures, near threshold, in the integral cross section were also found (possibly Feshbach resonances or Wigner cusps). However, more detailed calculations are required before any attempt to classify them might be made.

Try BSR and CCC



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