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Atomic collisional data for neutral beams and injected impurities in fusion plasmas

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Impurity seeding will be required for future reactors such as ITER and DEMO for radiative cooling, plasma control and diagnostics. Fusion plasmas are expected to contain impurities such as carbon, nitrogen, oxygen, argon, and tungsten ions. Some of these impurities are formed through ion seeding, others by erosion of plasma-facing components of the reactor. In the case of DEMO, due to the higher heating power required, highly charged impurities will be required to maintain the temperatures in the diverter region. Charge-exchange recombination spectroscopy (CXRS) is a diagnostic technique for measuring the impurity ion density, ion temperature, and plasma rotation within fusion plasmas [1]. The technique requires accurate state-resolved charge-exchange cross sections for collisions between seeded impurity ions and the neutral hydrogen beam injected during diagnostics and heating [2].

The wave-packet convergent close-coupling (WP-CCC) method can provide benchmark data on the total and state-selective cross sections for various processes taking place when fully stripped ions collide with atomic and molecular targets, see [3,4] and references therein. The approach is based on the expansion of the total scattering wave function using a two-centre pseudostate basis. This allows one to account for all underlying processes, namely, direct scattering and ionisation, and electron transfer into bound and continuum states of the projectile. The wave packets, constructed from the Coulomb waves, are used to discretise the continuum of the target and projectile atoms.

The WP-CCC approach has recently been extended to dressed-ion collisions with atomic hydrogen [5]. The method has been applied to calculate the total ionisation and state-resolved electron-transfer and target-excitation cross sections in C^{2+} and C^{3+} collisions with atomic hydrogen. The total electron-capture cross sections, calculated in a broad projectile energy range from 1 keV/u to 1 MeV/u, agree with available experimental and previous theoretical data. However, the results for ionisation overestimate the experimental data at the peak of the cross section supporting previous calculations.

Charge exchange in collisions of Ar^{16+} ions with hydrogen has also been investigated [6]. CXRS measurements performed at the ASDEX Upgrade [1] are based primarily on these impurities. For this projectile, capture into states with n=14–17, where n is the final-state principal quantum number, are found to be the most important. This is because the Lyman transitions from these states of Ar^{15+} are in the visible spectrum, which is well-suited for CXRS diagnostics. Experimental measurements are not available. Two different groups applied the classical trajectory Monte Carlo (CTMC) method for this system leading to very different results. We have calculated the state-resolved charge-exchange cross sections for n=6–19. For capture into the n=14–17 states a significant difference is observed between the present and previously published CTMC data. The cross sections differ by an order of magnitude within the most important energy range of 10–60 keV/u.

The WP-CCC method has also been applied to calculate various differential cross sections for ionisation in ion collisions with He [7] and H_2 [8]. Excellent agreement between the obtained results and the experimental data is found resolving longstanding discrepancies between theory and experiment. We review recent data relevant to fusion plasmas, obtained using the WP-CCC method.

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