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RESONANT ELECTRON SCATTERING BY METASTABE NITROGEN - REVISITED

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Abstract. Here we discuss the resonant electron scattering by a metastable nitrogen molecule in the $A^3\Sigma_u^+$ state, in particular the resonant electron impact quenching. This process was studied to some extent in the past but it has mainly been ignored in the recent nitrogen plasma modelling. The intention of this contribution is to draw attention to its potential importance. A classical local complex potential was used to evaluate cross sections for the vibrational excitation/de-excitation within the A-state vibrational manifold and for the resonant quenching of the $A^3\Sigma_u^+$ state to the $X^1\Sigma_g^+$ ground state.

1. INTRODUCTION

The modelling of nitrogen plasma has advanced significantly in its complexity in recent times due to various modern needs and improvements of modelling tools as well as updated data bases (e.g. see Loureiro et al., 2011). Pure nitrogen plasma has its fundamental importance for in-depth understanding of complex multitude of individual radiative and collisional processes among ions and neutral atoms and molecules and therefore it is a key test object for modelling techniques. However, a plasma of various gas mixtures, containing nitrogen has a much broader practical importance for understanding many phenomena in different environments ranging from planetary atmospheres (e.g. Campbell et al., 2010) to plasma processing. Enhanced interest in studies of the hydrogen – nitrogen plasma is recently present due to the needs of modelling the edge plasma in tokamak fusion reactors (Touchard et al., 2019). Nitrogen is introduced to the hydrogen (mainly its isotope, deuterium) plasma into the tokamak divertor region in order to enhance radiative dissipation of energy in this region. Production of ammonia occurs under such a condition and a corresponding detailed plasma modelling was performed (Carrasco et al., 2011; Sode et al., 2015; Body et al., 2018).

Among many of ionic, atomic and molecular electronic states of particles in a nitrogen containing plasma, the metastable $A^3\Sigma_u^+$ state of N_2 is often abundantly present. It plays a specific role due to the fact that it is the lowest triplet state and thus it is also populated by radiative decay of higher triplet states. It has long life-time, about 2s, and high excitation energy, 6.169 eV, between v=0 vibrational levels of $A^3\Sigma_u^+$ and ground $X^1\Sigma_g^+$ electronic states of N_2. Various processes involving N_2(A) are included in present time modelling and their relative relevance to the studied plasma depends on composition, pressure and temperature. Population of N_2(A) in p~1 Torr nitrogen discharge is strongly dependent on the excitation transfer between neutral molecules N_2(A), vibrationally excited ground state, N_2(X,v) and $N_2(B^3\Pi_g)$ (Loureiro et al., 2011). Nine different reactions in nitrogen involving N_2(A) are included in the modelling of Body et al., 2018. Also, the role of N_2(A) in the so-called breakdown memory effect in nitrogen was vividly discussed (e.g. Bošan et al., 1997, Petrović et al., 2001). Colonna and Capitelli, 2001 have shown strong influence of metastable nitrogen on characteristics of the electron energy distribution in a study of nitrogen expansion flow. They considered both, the atomic and molecular electronic metastable states and showed, that under studied conditions, the atomic species have more important role than the molecular ones. The superelastic collision of an electron with N_2(A) was shown to strongly influence the electron energy distribution during the post-discharge regime, Laporta, 2017.

Here, we are interested in electron collisions with a neutral nitrogen molecule which involves molecules in the lowest triplet state, $A^3\Sigma_u^+$.

2. ELECTRON IMPACT EXCITATION OF $A^3\Sigma_u^+$ STATE OF N_2

Electron collisions with a nitrogen molecule have been studied in detail since the very beginning of experimental and theoretical studies of atomic collision processes. A detailed overview of available data on e-N_2 collisions was presented by Itikawa (Itikawa, 2006) who also provided sets of recommended cross sections. The most detailed experimental differential cross sections (DCS) for excitation of this state, together with seven other states of N_2, were presented by the JPL group (Khakoo et al., 2005) for electron impact energies of 10, 12.5, 15, 17.5, 20, 30, 50, and 100 eV. The electron impact excitation of electronic states of nitrogen, including the $A^3\Sigma_u^+$ state, was also studied by *ab initio* calculations using the R-matrix technique by Gillan et al., 1996.

2.1 RESONANT EXCITATION

Resonances in electron molecule scattering are common phenomena when the incident electron is temporaly trapped to the target molecule and, on this way, allowing for increased energy exchange with molecule. The famous 2.3 eV resonance in nitrogen is the most studied prototype of shape resonances and it is produced by electron trapping to the ground electronic state of N_2 (e.g. Laporta et al. 2014). Similar resonances, core excited shape resonances, also occur when incoming electron is temporarily trapped in the potential of an excited molecular state. Such resonances are usually less pronounced than resonances associated to the ground electronic state of molecule because in this case two-electron transition is involved, trapping of the incoming electron and promoting a target electron to the excited orbital. Such core excited resonances associated to the $A^3\Sigma_u^+$ and $B^3\Pi_g$ state in nitrogen were first studied by Mazeau et al. 1973 and oscillatory structures in DCS were observed. Such structures are characteristic for resonance life-time being comparable to the vibrational period of the parent molecular state. The resonance in the excitation of $A^3\Sigma_u^+$ state which was attributed to the first excited $^2\Pi_u$ state of N_2^- was later studied in more detail by Paris group (Huetz et al.,1980a, b, c, and Čadež et al., 1986). It was also observed and commented by M. Allan in a review on electron impact excitation of triplet states (Allan, 1989). Our old relative experimental DCS for excitation of v=6 vibrational level of N_2(A) from Čadež et al., 1986, renormalized to the recent absolute DCS of Khakoo et al., 2005 at electron energy, Ee=10 eV are shown in Fig. 1. Absolute recommended total cross section (TCS) for excitation of N_2(A) from Itikawa, 2006 is also shown.

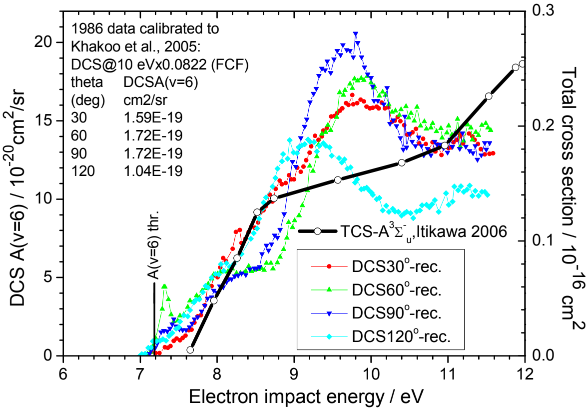

Figure 1: Renormalized DCS for excitation of the v=6 vibrational level of $A^3\Sigma_u^+$ at the 30°, 60°, 90° and 120° scattering angles from Čadež et al., 1986. Recommended absolute TCS for excitation of N_2(A) from Itikawa, 2006 is also shown.

It is important to note that resonant enhancement of the CS, unambiguously detected experimentally in v=6 DCS, does not show up in the TCS which is possibly due to a relatively small probability for the needed two electron transition in the incident reaction channel as commented in Allan, 1989 and also possibly due to the weaker Franck-Condon overlap with other then the v=6 vibrational level of N_2(A).

3. RESONANT ELECTRON SCATTERING BY $A^3\Sigma_u^+$ STATE

Even though the ~9.5 eV resonance, attributed to the $^2\Pi_u$ state of N_2^-, appears not to have an appreciable contribution to the excitation of N_2(A) by electron impact, its existence has potentially strong importance to processes involving $A^3\Sigma_u^+$ state in the discharges. An electron colliding with $N_2(A)$ can be more easily trapped to the $^2\Pi_u$ state of N_2^- as the $A^3\Sigma_u^+$ state is its parent state and, therefore, only one electron transition is involved, similarly to formation of the 2.3 eV $^2\Pi_g$ resonance in electron scattering by the ground state nitrogen. Besides this, the formation of a temporary $^2\Pi_u$ state of N_2^-, can importantly increase the electron impact quenching of $N_2(A)$ thus increasing the population of higher energy electrons in the electron energy distribution by this resonant superelastic channel which was also recently stressed out in Laporta, 2017. Both these aspects of the $^2\Pi_u$ were earlier treated in connection with processes in ionosphere (Čadež, 1983) using a local complex potential model for the resonance similar to the one used in Huetz et al., 1980. We are now re-examining the model by taking into account more accurate available potentials and some later theoretical development (e.g. Gianturco and Schneider, 1996).

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