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Modelling of Be transport in PISCES-B including metastable states

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Introduction. Beryllium (Be) will be used as plasma-facing material in the main chamber of ITER. The flux of eroded Be inside the tokamak will affect the plasma-surface interaction (PSI) processes in the carbon/tungsten divertor, which will finally determine the ITER duty cycle. Modelling is an important tool to make predictions for life time of divertor components and tritium retention in ITER [1]. ERO is a 3D Monte-Carlo (MC) impurity transport and PSI code, which also delivers resulting spectroscopy patterns. Alongside with application to ITER, it is important to verify the modelling assumptions and the underlying database including atomic data by ERO simulation of dedicated benchmarking experiments. For this, experiments with Be (seeded or sputtered from the target plate) at the linear plasma simulator PISCES-B (T_e~3÷10eV, n_e~1÷2*10^{12}cm^{-3}) have been modelled [2].

Effect of metastables. Among other parameters, the internal state of an atom, especially the population of metastable states (MS), affects the effective rates of excitation and ionization and, thus, light emission and transport through the plasma. Therefore, the separation of the 'atomic' and 'transport' part in the ERO modelling is challenging, except in case of homogeneous plasma. In an optimal way, at each point of the tracked Be particle trajectory a full collisional-radiative model (CRM) for Be should be applied. This is almost impossible in combination with MC approach due to amount of data and increase of calculation time. Therefore, often the CRM is reduced to one effective rate - photon emission coefficient (PEC) – which implies that the tracked species come instantly to an equilibrium with plasma. However, if a specie moves through plasma with high gradients of n_e and T_e, its internal state can be strongly affected by the local plasma parameters on its previous path. Also the initial population of levels (e.g. after physical sputtering) is an important issue.

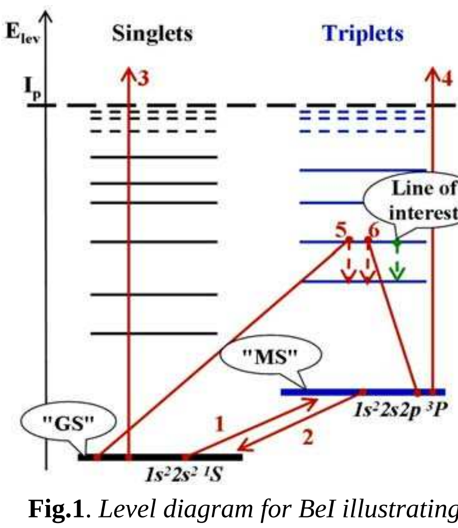

Fig.1. *Level diagram for BeI illustrating 6 effective rates used for tracking of one effective MS. 1,2 – transitions between MS and GS; 2,4 – ionization; 5,6 – contribution to light emission.*

In this work an intermediate approach is demonstrated on the example of tracking BeI *1s^{2}2s2p ^{3}P* state treated as an effective MS together with *1s^{2}2s^2 ^{1}S* ground state (GS) within ERO. In this case the population of triplet MS to a certain extent determines the ratio between triplet and singlet line intensities (fig.1).

Obviously, the relaxation time inside each of singlet and triplet systems is considerably smaller than the relaxation between them due to weak intercombinational transitions. The CRM is reduced to 6 effective rates (accumulation of all possible routes via levels; density dependence is captured from generalised collisional radiative theory) for transitions between MS and GS (“1”, “2”), ionization (“3”, “4”) from them and 2 effective photon efficiencies (“5”, “6”). The first 4 rates determine the relative population between MS and GS. The last couple of rates is individual for each line of interest.

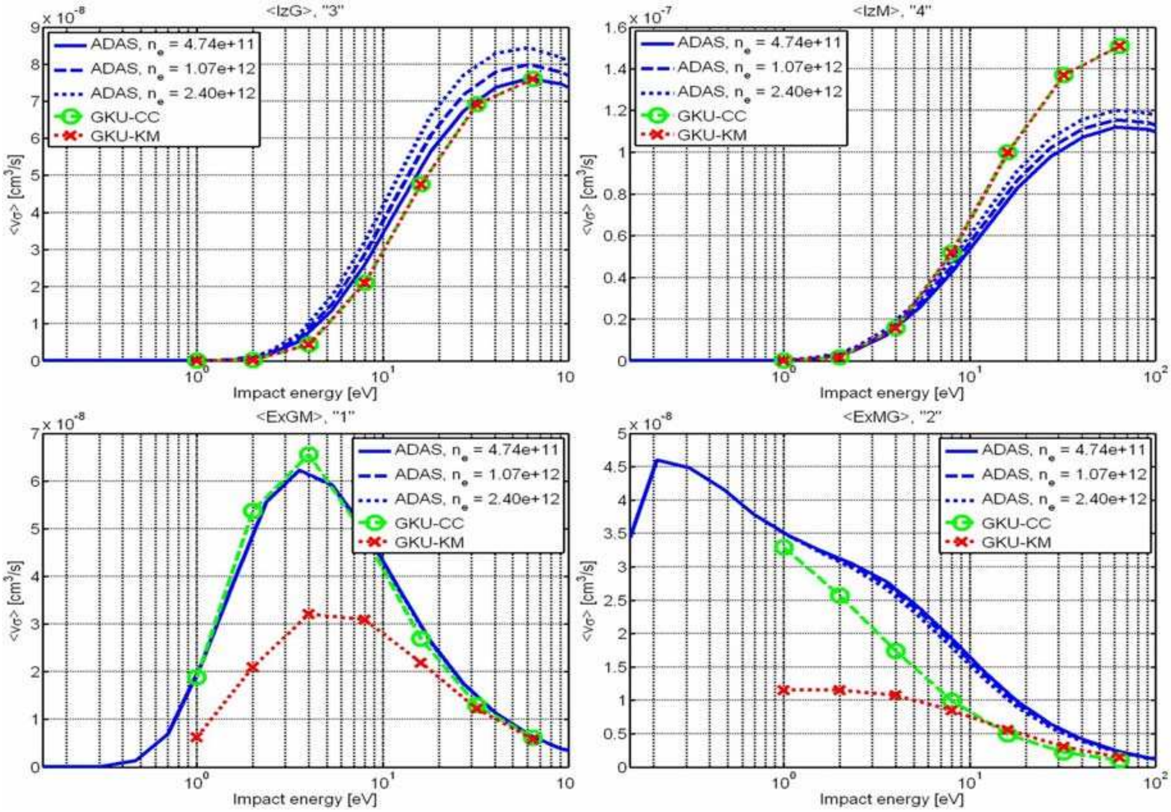

Fig.2. *Comparison of effective rates produced by ADAS and GKU. “<IzG>”,”<IzM>”- ionization from GS and MS; “<ExGM>” – transition GS→MS; “<ExMG>” – transition MS→GS. GKU code uses 2 sets of underlying data – calculated in K-matrix (“GKU-KM”) and CCC (“GKU-CC”) approaches.*

Atomic data. The mentioned effective rates for BeI are available from 2 sources – ADAS (Atomic Data and Analysis Structure) [3] and GKU code [4]. Fig. 2 shows the comparison of 4 effective rates (rates “1”-“4” from fig. 1). In GKU the dependence on electron density n_e is neglected, however the ADAS data has a weak dependence on n_e. In the case, if CCC-based (convergent close coupling) data set [5] for partial transitions is used in the GKU, it produces effective rates, which are in a good agreement with ADAS. The K-matrix [6] calculated data lead to the considerably lower GKU results for transitions between GS and MS. The reason for this discrepancy can be a topic for a separate discussion. It is probably worth to postpone the final judgement about the quality of the atomic data until the representative comparison with experiment (e.g. ERO simulations of PISCES-B experimental observations) will be available.

Populations in equilibrium – consistency check. The equilibrium relative population of MS and GS can be easily obtained from the balance equations if one assumes $dN_i/dt=0$, where N_i is level population. Fig. 3 illustrates the respective calculations. Here one can see the

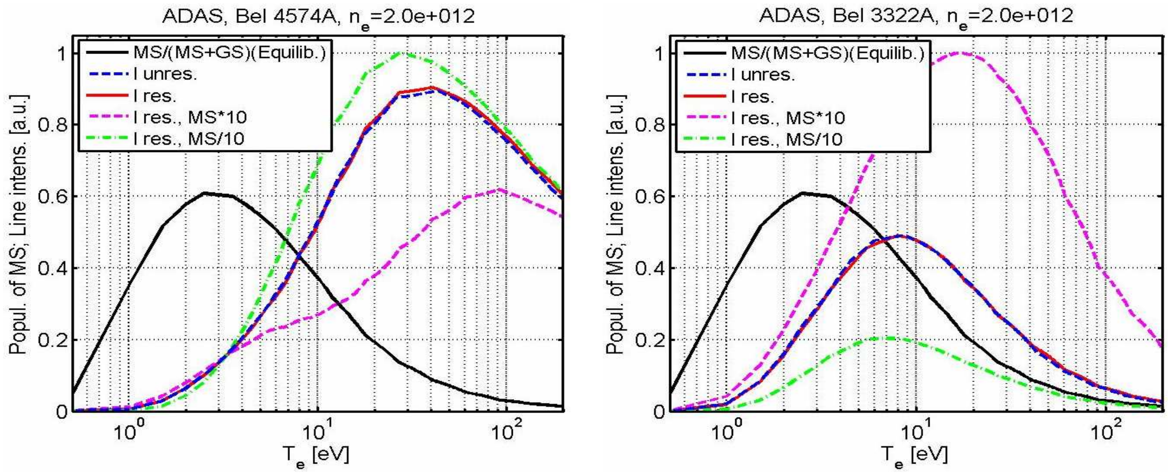

Fig.3. *'Equilibrium approach' illustration: relative MS population and respective line intensities in MS resolved ("I res.") and unresolved ("I unres.") cases; singlet (left) and triplet (right) lines.*

relative population of MS in equilibrium and the respective light intensities of the singlet (left) and the triplet (right) lines. As the MS resolved and unresolved data are produced from the same ADAS CRM, the assumption of equilibrium leads to the same line intensities ("I res.") as in case of single effective rate ("I unres."). The 2 curves, where MS population is artificially changed by a factor 10 ("MS*10", "MS/10") illustrate the possible effect of MS tracking. This effect is opposite for singlet and triplet lines, because for singlets most contribution comes from GS and for triplets from MS.

Dynamic approach. For MC calculations it is essential to calculate the change of MS/GS population during a single integration time step ***dt***. For the case of 1 MS tracking (2 balance equations) it is quite easy to get an analytical solution for $N_{GS}(t), N_{MS}(t)$. At low T_e, n_e the solution for normalized MS populations saturates at large ***t*** to the same value as in equilibrium calculations. At hotter and denser plasmas the ionization/recombination balance is important (the $N_{GS}+N_{MS}=1$ normalization is incorrect, because many Be particles are in the ionized state), so some deviations may arise. The equilibrium approach implies that recombination is in balance with ionization. The dynamic approach, neglecting recombination, is probably more adequate for PISCES-B, where Be is very effectively transported away from the plasma before recombining (most Be sticks to the wall).

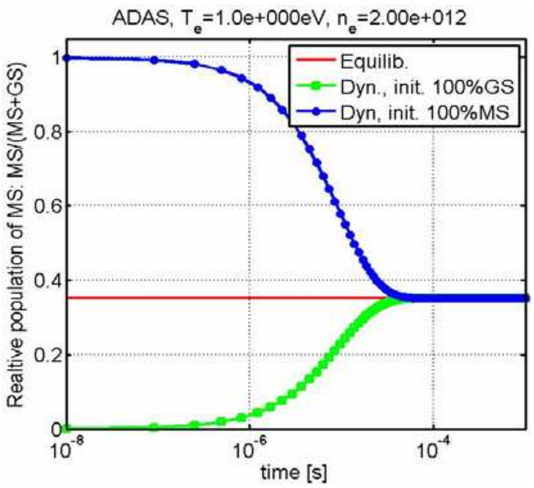

Fig.4. *Time evolution of MS population- "dynamic approach" ("Dyn.") with different initial conditions converging to the equilibrium approach obtained value ("Equilib.")*

Demonstration of MS tracking effect. The following dedicated case is useful to see the magnitude and direction of the MS tracking effect. Fig. 5 shows the calculation results for profiles along a narrow monoenergetic Be beam. In the 1st case (left) Be moves through a constant plasma. The MS population and thus, the ratio of triplet and singlet line intensities, converge to the same value for both extreme assumptions of initial full MS or full GS population, however it takes quite a significant

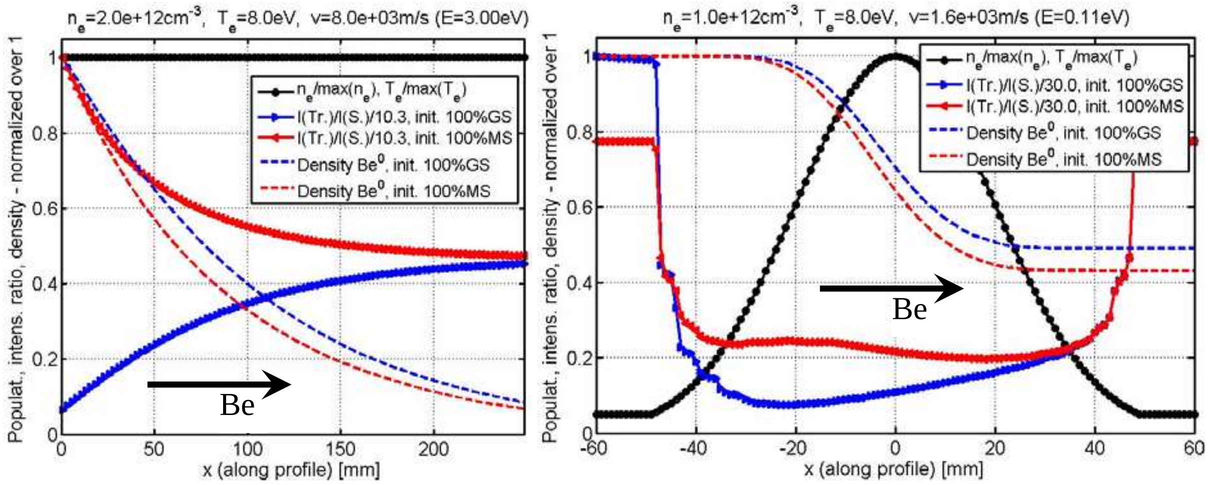

Fig.5. *Profiles along narrow monoenergetic Be beam. Constant (left) and Gaussian (right) background plasma profile. Ratio of triplet 3322A to singlet 4573A line ("I(tr.)/I(S.)") and neutral Be density for 2 extreme assumptions of initial population ("100%GS", "100%MS").*

distance of about 200mm. Until that ionization is different, because the contribution from MS is about 40% larger than from GS (fig. 2). In the 2nd case (right) the beam comes through Gaussian shaped plasma. The triplet to singlet ratio for different initial populations is about 3 times different at x=-20mm, where most of the BeI emission occurs. The ionization and, thus, the density of Be^0, after passing through the plasma also depends on the initial population. For maximal $n_e=2*10^{12}cm^{-3}$ the general picture remains similar, however the effect of initial population is less prominent, because relaxation between MS and GS happens faster. For both cases, the particle velocity is an essential parameter. In the 1st case an energy of E=3eV close to surface binding energy of Be was assumed, because it is relevant to the experiments at PISCES-B with sputtering from the Be target (Be moves mainly along the plasma column), and in the 2nd case E=0.11eV corresponds to 1300K temperature of the oven (oriented perpendicular to the plasma column) for the plasma seeding with Be [2]. It should be noted that, of course, the effect of MS tracking can be 'fogged' by interplay of many other effects and parameters such as the velocity distribution.

Conclusion. The tracking of even a single effective MS significantly improves MC simulation of not only light emission of plasma impurities, but also of their transport (due to influence on the ionization). The effect of MS is important if the MC test particle moves through plasma with high gradients of plasma parameters or if the MS population is affected by an additional process (physical sputtering, molecular decay, etc.). In the latter case MS tracking can be used to find a connection between those processes and the respective spectroscopic observations. The ERO modelling for PISCES-B spectroscopic experiments carried out previously [2] will be repeated using MS resolved approach.

References

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