3. WORKING GROUP REPORTS

3.1. Survey of atomic data base needs and accuracies for helium beam stopping and alpha particle diagnostics for ITER

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1. Introduction.

This report is concerned with establishing a recommended collection of atomic collision data for the modelling , experimental investigation and exploitation of helium beams. The initial and principal motivation stems from proposals for diagnostic beams for ITER, targeted at alpha particle measurement via double charge transfer/neutralised alpha analysis and spectroscopic analysis of recombination radiation. For the former, a 50keV/u helium beam is suggested and for the latter, a 100keV/u hydrogen beam. In the essentially abstracted exercise of atomic data judgement, it is necessary to avoid an over-restricted view of the requirements, particularly in collision energies. Evolution and modification of ideas is rapid in this field and will occur because of progress or lack of progress in beam development, because of information arising from existing fusion machines, and because of the linking of other beam/plasma validation experiments to the alpha particle detection task. In this respect, we note three points. Firstly beam emission spectroscopy (BES) and if possible charge exchange spectroscopy (CXS) should ideally be conducted in parallel with neutral particle analysis using the same (helium) beam. This maximises the mutual diagnostic support although strictly beam penetration and charge exchange state selectivity factors favour CXS with hydrogen beams. Secondly, evolution of related particle distribution functions such as slowing and thermalised alpha particles, the He^+ beam plume and the total helium inventory will be examined simultaneously with beam stopping and alpha particle source functions by modellers. Finally, models and the usefulness of the atomic data base will be assessed experimentally for some considerable period of time only on the present generation of machines. In this context, the JET experiment is particularly important since it is operating ^3He and ^4He beams at up to 55 keV/u and is commisioning neutral particle analysis, BES and CXS viewing these beams. The beams are the heating beams and therefore may allow assessment of minimum requirements for ITER diagnostic beams. In summary the helium data base should span possible ITER diagnostic beams and existing JET heating beams, enable alpha particle detection by neutral particle analysis and CXS, and support concommittant BES and CXS beam validation studies.

2. Beam energies, species and plasma conditions.

Detection of neutralised alpha particles using neutral helium beams depends on (i) penetration of the neutral helium beam to the point of collision with an alpha particle, (ii) neutralising of the alpha particle by double charge transfer, (iii) escape of the He^0 from the plasma for measurement. Since alpha particles are born by deuterium/tritium fusion at 880keV/u, this energy sets the upper limit for He^0 ion/atom stopping cross-sections. The lower limit is set by the beam He^0 particles in collision with thermal plasma ions. A beam energy ~30keV/u (JET ^4He beams) and plasma ion

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temperatures up to 30keV (15keV/u for D^+) would set ~1keV/u as the lower limit for ion/atom collision cross-sections. For ITER helium beams , which should certainly have particle energies ≥50keV/u, a lower energy limit for cross-sections ~10-20 keV/u is adequate. It should be noted that at 50keV/u, helium beams would only penetrate one quarter of the ITER minor plasma radius and not be capable of detecting central alpha particle sources.
Electron collisions contribute to beam stopping. Electron temperatures > 1keV corresponding to the low density plasma periphery, up to 25keV at the plasma core are relevant. However noting the sideline interest of HeI plasma edge emission for helium recycling and the helium inventory, and the present state of e/He^0 data, it is appropriate now to recommend cross-sections complete in energy from threshold to infinity.

Only fully ionised low and moderate mass ions, in collision with He^0 need to be considered. Of principal importance are the D^+, T^+ fuel and the He^{+2} ash or added minority. Other relevant impurities are due to choices of plasma facing first wall materials and then deposition and gettering strategies. This gives in order of importance C^{+6} (walls, X-point target plates, limiters, carbonisation), Be^{+4} (JET X-point target plates, limiters and evaporation) and B^{+5} (boronisation). The gettering procedures have reduced the importance of oxygen, but nontheless O^{+8} must be included. Other species are of less concern. Titanium, iron and nickel are possible structural materials, neon and argon useful added trace gases for diagnostics, and silicon a possible impurity. A representative set through the second and third period which would act as a basis for interpolation is Ne^{+10}, Si^{+14},Ar^{+18}, Fe^{+26}.

It is appropriate to make a broad statement of minimum accuracy requirements in cross-section data although more specific assessments are made in later contributions. Typically detector calibration, window transmission variation, spectral feature isolation and uncertainties in temperature and density profiles limit experimental accuracy to >40%, so this is the acceptable accuracy for modelling prediction of the final observed quantities. Therefore in beam driven diagnostics, 30% error in beam attenuation and 30% error in local particle production coefficients (eg. He^0 by neutralising) or photon effective emission coefficients (eg. by single charge transfer in CXS) calculation is acceptable. Beam attenuation up to a factor 10 is typically encompassed in an experiment, therefore net stopping cross-sections at <10% accuracy are required. Individual acceptable cross-section tolerances are then in inverse proportion to their contribution. Impurity cross-sections scale at worst as Z^2 and so their acceptable tolerances are in inverse proportion to Z^2 times the fractional impurity abundance. Helium fractional abundance at up to 20% may be expected in fusion plasmas, but experimental test plasmas of pure helium are possible. Carbon and light impurities at <5% are anticipated. The contribution of each impurity to Zeff is a helpful measure of its importance.

3. The required cross-section data

In presenting the following, it has been convenient to allow some repetition of cross-sections so that the different areas can appear complete. A coding (*1) - (*6) has been used to rank importance. A minimum accuracy is suggested with an indication of its variation with energy. For beam stopping, the accuracy is based on the proportion of each individual cross-section's contribution and its being the sole source of error. This is of course subject to revision in the light of improvement of our cross-section knowledge and progress in modelling. The lower limit for accuracy is set at 100%. Impurity cross-section accuracies are assessed as though the impurity alone is contributing. Zeff based adjustment of these as described in section 2 is appropriate. For electron collisions, for the reasons mentioned in section 2, 20% accuracy is suggested at all energies.

3.1. Alpha particle neutralisation

This is the essential reaction between beam He^0 and the alpha particle produced by deuterium/tritium fusion which allows the neutral particle diagnostics to probe the alpha particle sources.

He^{+2} neutralisation

(*1) $He^0(1^1S) + He^{+2} \rightarrow He^{+2} + He^0$,	20%

3.2. Beam and fusion He^0 stopping at low density

Most helium is in its ground state so that the dominant stopping is by electron loss directly from the ground state. If the plasma density is very low so that excited helium populations are negligible, this is the only pathway.

Ground state single electron loss with primary species and impurities

(*1) $He^0(1^1S) + D^+ \rightarrow He^+ + D^+ + e$,	87% @ 20keV/u, 13% @ > 100keV/u
(*1) $He^0(1^1S) + D^+ \rightarrow He^+ + D^0$,	11% @ 20keV/u, 42% @ > 100keV/u
(*1) $He^0(1^1S) + He^{+2} \rightarrow He^+ + He^{+2} + e$,	100% @ 20keV/u, 18% @ > 100keV/u
(*1) $He^0(1^1S) + He^{+2} \rightarrow He^{+1} + He^{+1}$,	16% @ 20keV/u, 20% @ > 100keV/u
(*2) $He^0(1^1S) + X^{+z} \rightarrow He^+ + X^{+z} + e$,	100% @ 20keV/u, 47% @ > 100keV/u
(*2) $He^0(1^1S) + X^{+z} \rightarrow He^{+1} + X^{+z-1}$,	12% @ 20keV/u, 19% @ > 100keV/u

[With the data at this stage, an approximate stopping can be obtained. However improvement at lower beam energies requires the following:]

Ground state double electron loss with primary species and impurities

(*2) $He^0(1^1S) + D^+ \rightarrow He^{+2} + D^+ + e + e$,	100%
(*2) $He^0(1^1) + D^+ \rightarrow He^{+2} + D^0 + e$,	100%
(*2) $He^0(1^1S) + He^{+2} \rightarrow He^{+2} + He^{+2} + e + e$,	100%
(*2) $He^0(1^1S) + He^{+2} \rightarrow He^{+1} + He^{+1} + e$,	100%
(*2) $He^0(1^1S) + He^{+2} \rightarrow He^{+2} + He^0$,	33% @ 20keV/u, 100% @ > 100keV/u
(*3) $He^0(1^1S) + X^{+z} \rightarrow He^{+2} + X^{+z} + e + e$,	83% @ 20keV/u, 44% @ > 100keV/u
(*3) $He^0(1^1S) + X^{+z} \rightarrow He^{+1} + X^{+z-1} + e$,	83% @ 20keV/u, 44% @ > 100keV/u
(*3) $He^0(1^1S) + X^{+z} \rightarrow He^{+2} + X^{+z-2}$,	100%

Ground state ionisation by electron impact

(*2) $He^0(1^1S) + e \rightarrow He^+ + e + e$,	20%

3.3. Beam and fusion He^0 stopping at moderate and high density

At plasma densities appropriate to ITER, impact excitation of helium from its ground state to excited states is sufficiently large for the latter populations to be non-negligible. Then electron loss from the excited states can occur before return to the ground. This enhances the stopping. The metastable state ($1s2s\ ^1S$ and $1s2s\ ^3S$) populations are the most important in this respect, so cross-sections involved in their formation and destruction are the first priority. Thereafter other excited state populations up to an effective cut-off principal quantum shell, at which Lorentz electric field or collisional merging to the continuum occurs, matter.

Ground state excitation to the n = 2 shell by primary species and impurities

(*2) $He^0(1^1S) + D^+ \rightarrow He^0(2^1S, 2^1P) + D^+$, 100%
(*2) $He^0(1^1S) + He^{+2} \rightarrow He^0(2^1S, 2^1P) + He^{+2}$, 100%
(*3) $He^0(1^1S) + X^{+z} \rightarrow He^0(2^1S, 2^1P) + X^{+z}$, 100%

Ground state excitation to the n = 2 shell by electrons

(*3) $He^0(1^1S) + e \rightarrow He^0(2^1S, 2^1P, 2^3S, 2^3P) + e$, 20%
[It is to be noted that ion impact excitations are spin system preserving, while electron collisions allow exchange]

n = 2 state single electron loss with primary species, impurities and electrons

(*2) $He^0(2^{2S+1}L) + D^+ \rightarrow He^+ + D^+ + e$, 100%
(*2) $He^0(2^{2S+1}L) + D^+ \rightarrow He^+ + D^0$, 100%
(*2) $He^0(2^{2S+1}L) + He^{+2} \rightarrow He^+ + He^{+2} + e$, 100% (includes inner electron ionisation)
(*2) $He^0(2^{2S+1}S) + He^{+2} \rightarrow He^{+1} + He^{+1}$, 100%
(*3) $He^0(2^{2S+1}L) + X^{+z} \rightarrow He^+ + X^{+z} + e$, 100% (includes inner electron ionisation)
(*3) $He^0(2^{2S+1}S) + X^{+z} \rightarrow He^{+1} + X^{+z-1}$, 100%
(*3) $He^0(2^1S, 2^1P, 2^3S, 2^3P) + e$ --> $He^+ + e + e$, 20%

Redistributive collisions within the n = 2 shell by primary species, impurities and electrons

(*2) $He^0(2^{2S+1}L) + D^+ \rightarrow He^0(2^{2S+1}L') + D^+$, 100%
(*2) $He^0(2^{2S+1}L) + He^{+2} \rightarrow He^0(2^{2S+1}L') + He^{+2}$, 100%
(*3) $He^0(2^{2S+1}L) + X^{+z} \rightarrow He^0(2^{2S+1}L') + X^{+z}$, 100%
(*3) $He^0(2^{2S+1}L) + e \rightarrow He^0(2^{2S+1}L') + e$, 20%
[With the data at this stage, the 2^1S state populations and enhanced stopping via the singlet side can be obtained approximately. The 2^3S state population is incorrect and requires the following:]

Ground state excitation to the $2 < n \leq 4$ shells by primary species and impurities

(*3) $He^0(1^1S) + D^+ \rightarrow He^0(n^1L) + D^+$, 100%
(*3) $He^0(1^1S) + He^{+2} \rightarrow He^0(n^1L) + He^{+2}$, 100%
(*4) $He^0(1^1S) + X^{+z} \rightarrow He^0(n^1L) + X^{+z}$, 100%
[It is to be noted that excitation to 4^1F opens access to the triplet side through state mixing with 4^3F]

Ground state excitation to the $2 < n \leq 4$ shell by electrons

(*3) $He^0(1^1S) + e \rightarrow He^0(n^1L, n^3L) + e$, 20%

$2<n\leq 4$ state single electron loss with primary species, impurities and electrons

(*3) $He^0(n^{2S+1}L) + D^+ \rightarrow He^+ + D^+ + e$,	100%
(*3) $He^0(n^{2S+1}L) + D^+ \rightarrow He^+ + D^0$,	100%
(*3) $He^0(n^{2S+1}L) + He^{+2} \rightarrow He^+ + He^{+2} + e$,	100% (includes inner electron ionisation)
(*3) $He^0(n^{2S+1}S) + He^{+2} \rightarrow He^{+1} + He^{+1}$,	100%
(*4) $He^0(n^{2S+1}L) + X^{+z} \rightarrow He^+ + X^{+z} + e$,	100% (includes inner electron ionisation)
(*4) $He^0(n^{2S+1}L) + X^{+z} \rightarrow He^{+1} + X^{+z-1}$,	100%
(*4) $He^0(n^{2S+1}L) + e \rightarrow He^+ + e + e$,	20%

Redistributive collisions between $2\leq n,n'\leq 4$ shells by primary species, impurities and electrons

(*3) $He^0(n^{2S+1}L) + D^+ \rightarrow He^0(n'^{2S+1}L') + D^+$,	100%
(*3) $He^0(n^{2S+1}L) + He^{+2} \rightarrow He^0(n'^{2S+1}L') + He^{+2}$,	100%
(*4) $He^0(n^{2S+1}L) + X^{+z} \rightarrow He^0(n'^{2S+1}L') + X^{+z}$,	100%
(*4) $He^0(n^{2S+1}L) + e \rightarrow He^0(n'^{2S+1}L') + e$,	20%

Residual cross-sections up to $n=10$ by primary species, impurities and electrons

(*5) $He^0(n) + D^+ \rightarrow He^0(n') + D^+$,	100%
(*5) $He^0(n) + He^{+2} \rightarrow He^0(n') + He^{+2}$,	100%
(*6) $He^0(n) + X^{+z} \rightarrow He^0(n') + X^{+z}$,	100%
(*5) $He^0(n) + e \rightarrow He^0(n') + e$,	20%

[Spin system merging and l-subshell mixing is large beyond $n=4$ and merging with the continuum by field ionisation occurs by $n=10$ typically.]

3.4. Beam emission spectroscopy

Spectral emission from the beams is an important opportunity for experimental verification of beam attenuation and of the correctness of the enhancements attributed to the finite plasma density. Exploitation of the scope of beam emission spectroscopy dictates that emission from helium excited states up to the $n=4$ shell should be modelled carefully. For example the transitions $4\,^1L - 2\,^1P$ are of particular interest since the forbidden components and linear Stark shifts are diagnostic. The overall atomic data requirements are the same as for beam stopping at moderate and high density. However the priority and accuracy for processes populating and depopulating upper states of observable spectrum lines are altered. These are repeated here.

Ground state excitation to the $2<n\leq 4$ shells by primary species and impurities

(*2) $He^0(1^1S) + D^+ \rightarrow He^0(n^1L) + D^+$,	30%
(*2) $He^0(1^1S) + He^{+2} \rightarrow He^0(n^1L) + He^{+2}$,	30%
(*2) $He^0(1^1S) + X^{+z} \rightarrow He^0(n^1L) + X^{+z}$,	30%

Ground state excitation to the $2<n\leq 4$ shell by electrons

(*2) $He^0(1^1S) + e \rightarrow He^0(n^1L, n^3L) + e$, 20%
[Initial estimates suggest that 4^1L - 2^1P on the singlet side and 3^3P - 2^3S on the triplet side should be studied experimentally.]

$2<n\leq4$ state single electron loss with primary species, impurities and electrons

(*2) $He^0(n^{2S+1}L) + D^+ \rightarrow He^+ + D^+ + e$, 36% @ 20keV/u, 36% @ > 100keV/u
(*2) $He^0(n^{2S+1}L) + D^+ \rightarrow He^+ + D^0$, 100%
(*2) $He^0(n^{2S+1}L) + He^{+2} \rightarrow He^+ + He^{+2} + e$, 36% @ 20keV/u, 39% @ > 100keV/u (includes inner electron ionisation)
(*2) $He^0(n^{2S+1}L) + He^{+2} \rightarrow He^{+1} + He^+$, 49% @ 20keV/u, 100% @ > 100keV/u
(*3) $He^0(n^{2S+1}L) + X^{+z} \rightarrow He^+ + X^{+z} + e$, 42% @ 20keV/u, 32% @ > 100keV/u (includes inner electron ionisation)
(*3) $He^0(n^{2S+1}L) + X^{+z} \rightarrow He^+ + X^{+z-1}$, 100%
(*3) $He^0(n^{2S+1}L) + e \rightarrow He^+ + e + e$, 20%

Redistributive collisions between $2\leq n,n'\leq4$ shells by primary species, impurities and electrons

(*2) $He^0(n^{2S+1}L) + D^+ \rightarrow He^0(n'^{2S+1}L') + D^+$, 30%
(*2) $He^0(n^{2S+1}L) + He^{+2} \rightarrow He^0(n'^{2S+1}L') + He^{+2}$, 30%
(*3) $He^0(n^{2S+1}L) + X^{+z} \rightarrow He^0(n'^{2S+1}L') + X^{+z}$, 30%
(*3) $He^0(n^{2S+1}L) + e \rightarrow He^0(n'^{2S'+1}L') + e$, 20%

3.5. Charge exchange spectroscopy

State selective single electron charge transfer from neutral helium beam atoms in their ground state to alpha particles forming excited states of He^{+1} is the initial concern. Subsequent HeII emission, such as n=4-3 at 4685A, is the CXS signal to be contrasted with the neutral particle analyser signals. There is a futher aspect however , in that, neutral helium beams may be useable in CXS for all light impurity densities. Consistency with impurity densities used for modelling beam stopping may then be sought.

State selective charge transfer from ground state to primary species

(*2) $He^0(1^1S) + He^{+2} \rightarrow He^+ + He^+(nl\,^2L)$, 30%
(*2) $He^0(1^1S) + D^+ \rightarrow He^+ + D(nl\,^2L)$, 30%
[The first is the key reaction for CXS. The second is relevant for formation of the D^0 halo associated with the helium beams. For He, $1\leq n\leq6$, and for D, $1\leq n\leq4$, are relevant ranges.]

State selective transfer ionisation from ground state to primary species

(*4) $He^0(1^1S) + He^{+2} \rightarrow He^{+2} + He^+(nl\,^2L) + e$, 100%
(*4) $He^0(1^1S) + D^+ \rightarrow He^{+2} + D(nl\,^2L) + e$, 100%
[These reactions tend to populate low n shells. They provide a correction of CXS using short wavelength transitions.]

State selective charge transfer from metastables to primary species

(*4) $He^0(2^1S, 2^3S) + He^{+2} \rightarrow He^+ + He^{+1}(nl\ ^2L)$, 100%
(*4) $He^0(2^1S, 2^3S) + D^+ \rightarrow He^+ + D(nl\ ^2L)$, 100%
[These reactions are most relevant at low beam energies and to CXS with visible lines since the dominant receiving n-shell is usually close to the line emitting n-shell. Expectations of beam metastable populations suggest this is only a modest correction. For He, $1 \leq n \leq 6$, and for D, $1 \leq n \leq 4$, are relevant ranges.]

State selective charge transfer from ground state to impurities

(*3) $He^0(1^1S) + X^{+z} \rightarrow He^+ + X^{+z-1}(nl\ ^2L)$, 30%
[This allows a full CXS diagnostic for impurities using helium beams. The relevant range is $1 \leq n \leq 2z^{0.75}$.]

4. Conclusions

We have sought to lay out the set of atomic collision cross-section data required to model and support alpha particle diagnostics for ITER using neutral helium beams. However, we have gone further in that we have also addressed the data required in practise to support and validate such a diagnostic fully. It is anticipated that the data will form the high quality input to comprehensive excited population, effective ionisation coefficient and effective emissivity coefficient codes in the collisional-radiative sense. There remain some anxieties. As has been mentioned, fast neutral helium atoms in tokamak plasmas will experience a strong vxB electric field establishing a Stark state structure. Whether this can alter the balance of atomic reactions significantly is largely unexplored. Also assumptions of isotropic averages of collision cross-sections cannot really be sustained. We therefore anticipate some elaboration or at least clarification of these points.