Comparison of charge transfer in proton collisions with methane and silane for simulations of divertor impurities and technological plasmas

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Silane and methane are useful gasses for diagnostics of impurity deposition and implantation, as recently reported in case of the scrape off layer of inner divertor [1]. Hydrocarbons including methane naturally occur when graphite is used as plasma facing material; silane is used not only for fusion plasma diagnostics, but silane plasmas are also of key interest in the semiconductor industry. The data need for accurate charge transfer cross sections in proton collisions with both molecules has been stated in the series of Juelich reports by Janev and Reiter [2], who provide semi-empirical formulas for charge transfer in collisions of proton with CH_4,

$$\sigma_{CX} = \frac{9.96}{\sqrt{E} + 85E^{2.5}} + \frac{30.2}{E^{0.015} + 9.0\times10^{-6}E^{1.2} + 2.19\times10^{-18}E^{3.8} + 4.47\times10^{-22}E^{4.4}} (10^{-16} cm^2)$$

and for charge transfer in collisions of proton with SiH_4,

$$\sigma_{CX} = \frac{3.93}{\sqrt{E} + 445E^{2.3}} + \frac{46.2}{E^{0.094} + 9.0\times10^{-6}E^{1.2} + 2.845\times10^{-18}E^{3.8} + 5.81\times10^{-22}E^{4.4}} (10^{-16} cm^2)$$

respectively (energy E is given in units of eV).

Here we compare the above formulas with previous cross sections results on methane [3] and new results on silane, based on multi-reference single- and double-excitation configuration interaction (MRD-CI) calculation of electronic structure of collision intermediates, and molecular orbital close coupling calculation (MOCC) of electron capture dynamics. Figure 1 shows the electron capture cross section for H^+/SiH_4 collision.

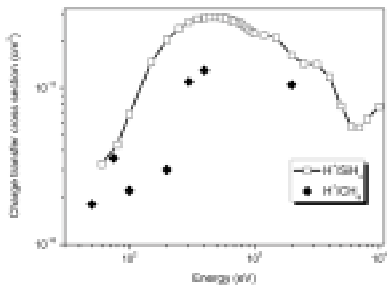

Fig. 1: Cross sections for proton-impact charge transfer

Implications for plasma impurity simulations and energy balance in low-temperature regions on the wall of fusion reactors will also be discussed at the conference.

[1] J. Likonen, S. Lehto, J. P. Coad, et al., "*Studies of impurity deposition/implantation in JET divertor tiles using SIMS and ion beam techniques*", Fusion Engineering and Design **66** (2003) 219-224.
[2] R. Janev and D. Reiter, Institut fur Plasmaphysik, Forschungszentrum Juelich, Juel-Report 3966 and Juel-Report 4038, 2002.
[3] M. Kimura, Y. Li, G. Hirsch, and R. J. Buenker, Physical Review A 52, 1197-1204 (1995).