Model Calculations of Ion Induced Desorption Yields \diamond

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The ion induced desorption is a severe luminosity limitation for low charge state heavy ion accelerators. Therefore, it was intensively investigated in dedicated experiments during the last years. It was shown that the ion induced desorption is a surface effect with a strong link to the substrate [1]. The overall quantity of desorbed gas during long term irradiation is always in the range of a monolayer $(10^{15} \text{ cm}^{-2})$. From the geometrical cross section of the projectile desorption yields of $\eta \geq 100$ molecules per incident ion cannot be explained. Therefore we have developed a theoretical model to describe the ion induced desorption as a thermally driven process using the inelastic Thermal Spike Model.



<u>Fig. 1</u>: Temperature evolution of the electronic system (top) and the lattice (bottom)

The inelastic Thermal Spike Model has been developed to explain the processes of track formation and sputtering induced by heavy ions in energy ranges where the electronic energy loss is dominating [2]. First the projectile energy is deposited in the electronic subsystem of a sample. The hot electrons distribute the energy radially away from the ion path within typically 10^{-15} s. Especially in metals the free electrons moderate the energy deposition. After around 10^{-13} s the electronic system heats the lattice by electron-phonon coupling and after 10^{-10} s the sample approaches ambient temperature again. A computer code to calculate the time dependent radial evolution of the temperature of the electronic system as well as the lattice of metals was developed years ago. We have extended this code to describe the ion induced desorption as a thermally moderated process in terms of

$$\frac{\partial^2 \eta}{\partial r \partial t} = \nu_0(T(r,t)) \cdot \tilde{n}(r,t) \cdot exp\left(-\frac{E_{des}}{k_B \cdot T(r,t)}\right) \qquad (1)$$

where $\nu_0(T(r, t))$ is the oscillation frequency of the bound molecules, $\tilde{n}(r, t)$ is the surface coverage and the exponential term the number of the adsorbats that overcome the binding energy given by the Boltzmann distribution.

In figure 1 the temperature evolution in space and time of a copper sample after a 1.4 MeV/u Xe impact is shown for the electronic and the lattice system. The influence of the ion impact is even visible in some 10 nm.



Fig. 2: Desorption from one single projectile

This transient overheated spot leads to an enhanced thermal desorption shown in figure 2. Here the desorption per time is plotted against the circle segment of a certain radius. The most gas is desorbed from a radius of some nm around the projetiles impact and not from r = 0, where the highest temperature is reached but the total surface coverage is minimal. Some example values are compared to experimental numbers in the table to give an impression of the results of the calculation. Even the experimentally found $(dE/dx)^2$ -scaling is reproduced by the model.

Proj. $(1.4 MeV/u)$	Xe	Xe	Xe	С	Pb	Pb $(4.2 \mathrm{MeV}/\mathrm{u})$
Target	Cu	Au	Rh	Cu	Cu	Au
Experiment	290	90	1280	10	800	800 (prel.)
Calculation	185	165	3400	5	525	750

In conclusion the extended inelastic Thermal Spike Model is the first approach to calculate ion induced desorption yields in the investigated energy regimes. As measured in numerous experiments gold and copper show also the lowest desorption yields in the calculation and will thus be used as beam loss collimator materials.

References

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[2] Z.G. Wang et al., J. Phys.:Condens. Matter 6 (1994) 6733

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