STORAGE RING BAKE-OUT EFFICIENCY FROM THE ACCELERATOR PARAMETERS POINT OF VIEW

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Abstract

In the past, it was generally believed that carefully performed in-situ bake-out of the storage ring vacuum chamber can lead to a lower photon induced desorption and subsequently to a longer beam lifetime. At a later stage of the machine life, some labs (among them ELETTRA) have eliminated bake out. It will be shown that during bake-out up to 450 ˚C only molecules with low sorption energy can be desorbed. Photon stimulated desorption can also remove tightly bounded molecules which are always present on technological surfaces. The high efficiency of beam cleaning depends on the critical energy of photons. The desorption yield coefficient as well as necessary conditioning time can be estimated knowing the bending magnet intensity.

1 ELETTRA OPERATIONAL EXPERIENCE

The first beam in ELETTRA was circulated in October 1993. Before start up the static pressure in the vacuum chamber varied from $2x10^{-8}$ mbar to $6x10^{-10}$ mbar. The lowest pressure was achieved in the III. vacuum sector, where the bake out procedure at 150 ˚C was partially carried out (straight sections and crotches were only heated). At this vacuum condition commissioning proceeded and 165 mA@1 GeV were stored. After about 0.7 Ahours of integrated current the total pressure in all vacuum sectors achieved the low 10^{-9} mbar range. The water peak dominant in the residual gas mixture before start up, decreased in the whole ring to the 10^{-10} mbar range. The II. vacuum sector was then in situ baked and the beam current of 410 mA@1 GeV was reached.

The remaining sectors of the ring were baked successively during various shutdown periods. On two occasions it happened that the bake out cycle started at quite acceptable pressure in the ring, but after bake out the pressure increased up to 10^{-4} mbar range due to some leaks opened during the cooling of the chamber.

In all these cases conditioning of the vacuum chamber proceeded well and after 27 Ahours of dose the beam currents of 10 and 70 mA@2.3 and 1.5 GeV, respectively, were stored. The total pressure decreased to the low 10^{-10} mbar range and the residual gas mixture was dominated by hydrogen peak (~95%) and carbon monoxide peak (~4%), C, CO_2, H_2O and CH_4 peaks had a proportional very low level as is typical for the clean vacuum system.

In fact, ELETTRA commissioning started with incomplete in-situ bake out. Moreover, during commissioning a number of events occurred that are relevant to the vacuum conditions: more than 70% of storage ring vacuum chambers had to be opened to replace the faulty gaskets of all RF cavities, at least one vacuum sector had to be vented to install photon absorbers or beam stoppers, the whole ring was vented, sector per sector, when the modified beam position monitor gaskets were installed. The bake out procedure was never carried out after these interventions. The base pressure without beam was routinely obtained in the high 10^{-9} mbar range and the operation pressure in the high 10^{-10} mbar range (250 mA@2 GeV) was reached, as well.

Daresbury laboratory reported similar experience, where after machine upgrade no bake out has been carried out [1].

The elimination of in situ bake out can overcome such problems as thermal stress, in our case resulting in opening of leaks after cooling. The in situ bake out is also enormly time consuming (as a minimum 1 week per vacuum sector). Moreover, magnets with lower gaps can be installed.

It will be very useful, especially for the new projects, to explain the elementary process of sorption which occur on the vacuum chamber surface. Combining theoretical approach and experimental observation the new and more scientific conclusions can be made on bake out necessity.

2 THEORETICAL AND EXPERIMENTAL ASPECTS OF ADSORPTION/DESORPTION PROCESSES

When gas molecules are in contact with a surface which is capable to adsorb them, the amount of gas molecules decreases and gas molecules are trapped on the surface. This process can be also inverted (desorption) and at the suitable conditions the equilibrium is established. From a thermodynamic point of view this process can be characterised by the adsorption/desorption Eyring's rate constant:

$$\mathbf{k_{ads/des} = \frac{kT}{h}\frac{f^{+}}{f_A f_S}\exp\{-\frac{E^{+}_{ads/des}}{RT}\}}$$

where k, h, R are the Boltzmann's, Planck's and the gas constants, respectively, T is a surface temperature, $E_{ads/des}^{+}$ is the activation energy of adsorption/desorption, f_S, f_A, f^{+}, are partition function of the surface S, gas molecule A and activated complex (+), respectively. If the total product of partition functions is near to 1, the activation energy plays a decisive role in adsorption/desorption processes. The value of activation energy is determined by the character of interaction forces between a surface and gas molecule on the "reaction path". To evaluate the activation energy of adsorption/desorption theoretical as well as experimental approaches can be used.

2.1 Theoretical Calculations of Activation Energies

The activation energy of adsorption/desorption can be calculated applying the method of the empirical potentials. This method can be used when in the interaction of two systems the long range forces are dominant (e.g. physisorption, polar sorption or low energy chemisorption). In this approach the total interaction energy E can be expressed as a sum of dispersion E_D, repulsion E_R, induction E_I and coulomb E_C terms:

$$E = E_D + E_R + E_I + E_C$$

The dispersion term is expressed [2]:

$$E_D = -\sum_i \sum_j C_{ij}\, r_{ij}^{-6}$$

C_{ij} is the dispersion attraction constant, r_{ij} is the distance from the surface atom i to the gas molecule atom j. The attraction constant can be calculated according to the Kirkwood-Muller or Slater-Kirkwood formula [3], [4].

The repulsion part of interaction can be calculated as [3]

$$E_R = \sum_i \sum_j B_{ij}\, r_{ij}^{-12}$$

The induction part of the total energy can be approximated as

$$E_I = \sum_j \frac{\alpha_j}{2}\, \varepsilon_j^2(r)$$

where α_j is the polarizability of the gas molecule atoms and ε_j (r) is intensity of the electrostatic field created by charges of the surface atoms.

The electrostatic (coulomb) term is given by interaction between the charge distribution on the surface (q_i) and the charge distribution on the gas molecule (q_j)

$$E_C = \frac{1}{4\pi\varepsilon_o} \sum_i \sum_j \frac{q_i q_j}{r_{ij}}$$

The method of empirical potential is the simplest method that can be used to calculate adsorption/desorption energy of the gas molecules on the surface. If in the interaction short range forces are not negligible the quantum mechanical approach must be used.

In quantum mechanical calculations of interaction energies between surfaces and gas molecules the Schrodinger's equation is solved

$$\hat{\mathbf{H}}\psi = \mathbf{E}\psi$$

where Ψ is the wave function and the total Hamilton's operator $\hat{\mathbf{H}} = \hat{\mathbf{H}}^A + \hat{\mathbf{H}}^S + \hat{\mathbf{H}}^U$. $\hat{\mathbf{H}}^A$ and $\hat{\mathbf{H}}^S$ are the total hamiltonians corresponding to the systems A and S, respectively, $\hat{\mathbf{H}}^U$ is the operator including all intermolecular interactions. Schrodinger's equation can be solved by variation or perturbation methods.

The use of variation method on calculations of adsorption/desorption energies is a problem. All methods are based on Hartree-Fock's method which in principle cannot describe the dispersion (attraction) energy. This problem can be overcome applying the SCF (self-consistent field) methods widely used to calculate simple models of adsorption.

While short and middle range forces are dominant (e.g. strong chemisorption) the overlap between interacting systems is not negligible. Therefore, the antisymetrized product of the wave function $\Psi = A\ \Psi^A \Psi^S$ must be considered. *A* is the antisymetrizator which guarantees that the wave function is antisymetric for the electrons exchange.

The first order perturbation method of calculations leads to the classic coulomb interaction that can be attractive or repulsive. The second order perturbation calculations lead to the inductive and dispersive interaction.

All above described methods are used to calculate theoretically the adsorption/desorption energies between surfaces and gas molecules. Until now, theoretical values of sorption energies were only published for surfaces like zeolites, non evaporable getters, silicagel etc. In these cases the crystallographic structure of the surface is well known. Industrial surfaces of the stainless steel or aluminium are amorphous ones. At first it is necessary to find the appropriate theoretical model of these surfaces and then the previously described methods of calculation can be applied. Anyway, from individual terms of the interaction energy can be seen that the character of forces between the surface atoms and gas atoms plays a decisive role and no "memory effect" should be considered.

2.2 Experimental Determination of Adsorption/Desorption Energy

There are many experimental method suitable to measure sorption energies. One of the most suitable methods is the method of thermal desorption spectroscopy (TDS). In this method the surface is placed in a pumped vacuum system and successively heated to the desired temperature. From the desorption spectrum, i.e., the dependence of pressure changes on the temperature of the surface, activation energies of desorption E can be evaluated.

The desorption rate dn/dt (n is the surface concentration, t is time) is given by Arrhenius' equation:

$$-\,dn/dt = n^x \nu_x \exp\{-E/RT\}$$

ν is the vibration factor, x is the reaction order (1 or 2). The surface temperature increases from the initial temperature T_0 according to the formula: $T = T_0 + a.t$, a is a heating rate. From the temperature T_m at which the desorption rate is a maximum, the activation energy of desorption can then be calculated iteratively according to the equation

$$1/T_m (1 + E/RT_m) = kT_m/ha \exp\{-E/RT_m\}$$

It can be shown that in wide ranges of temperatures and heating rates the activation energy of desorption can be approximated by formula

$$E = 70\ T_m\ [\text{cal/mol}] = 300\ T_m\ [\text{J/mol}]$$

Using this approximation values of desorption energy can be simply calculated.

3 EFFICIENCY OF BEAM CLEANING AND CONCLUSIONS

TDS formulas can be applied for describing bake out processes used for surface treatment of vacuum chambers.. The highest the maximum heating temperatures are the highest activation energies of desorption can be achieved as is summarised in Table 1:

Table 1: Heating temperatures and corresponding energies

T [˚C]	150	300	900
E [eV/mol]	8e23	1e24	2e24

On the other hand, the inner surface of the storage ring vacuum chamber is during machine operation exposed to synchrotron radiation. Photons of the wide range of wavelengths are hitting the external part of the bending magnet chamber. By means of photodesorption gas molecules previously trapped on the surface can be eliminated and pumped. The efficiency of photodesorption depends on the energy of photons

$$E = h.\nu = h.c/\lambda$$

ν, λ are the photon's frequency and wavelength, respectively, c is the light speed.

In Table 2 are summarised wavelengths from visible to X-ray photons and corresponding energies

Table 2: Light wavelengths and corresponding photons' energies

λ [nm]	500	200	1
E [eV/mol]	4e26	8e26	2e27

Comparing energy values reachable during bake out with energies of the visible, ultraviolet or X-ray photons is clear that the light energies are much higher. It means that high energy photons can cause also desorption of tightly bounded molecules which are always present on the industrial surfaces.

This theoretical presumption was also confirmed during ELETTRA commissioning and operation. Pressures with beam in the freshly installed chambers increased up to 10^{-7} mbar range equally for in situ baked as well as for non baked vacuum vessels. It means that only the few weakly bonded molecules can be eliminated during thermal surfaces treatments.

There is still the open question which part of the chamber is exposed to radiation and how wall conditioning of chamber parts not directly hit by photons proceeds. Several processes should be considered to explain beam cleaning efficiency: i) secondaries effect, ii) reflected photons passing through the slots, iii) characteristic radiation emitted by surfaces exposed to primary photons (e.g. copper absorbers). Energies of characteristic radiation are sufficient not only to ionise residual gas molecules but can lead to photodesorption. In all these cases the angle of incidence should be taken into account. In those cases the angle of incidence is unfavourable the process of surface migration should be considered which assures that surface concentration equilibrium will be established. After a proper conditioning time the homogeneously clean surface is obtained.

The necessary conditioning time can be estimated from the known numbers of emitted photons per meter of irradiated bending magnet chamber per one Amp hour of dose D and from the corresponding value of desorption yield coefficient η. The number of photons emitted per meter N_y can be simply calculated from the formula [5]

$$N_y\ [\text{phot/m}] = 1.4 \times 10^{23}\ B\ [T]\ D[Ah]$$

where B is the bending magnet field intensity in Tesla. The corresponding values of coefficient η for different materials (SS, Cu, Al) can be taken from ref. [6].

At ELETTRA 1 Ahour of dose corresponds to 1.7×10^{23} phot/m. Vacuum chamber conditioning proceeds rapidly and the in situ bake out has been eliminated. For the same reason the bake out procedure is no more repeated at KSRS [7] and for the newest projects of the third generation synchrotron light sources (e. g. ANKA [8], SLS [9]) the non bake out start up is being considered.

REFERENCES

[1] Suller V.: private communication

[2] Born M., Mayer J. E.: Z. Physic. 75, 1 (1932)

[3] Kirkwood J. G.: Phys Z., 33, 57 (1932)

[4] Muller A: Proc. Royal Society A, 154 625 (1936)

[5] Walker R. P.: Proc. 5th CAS Gen. Accel. Physic Course, CERN 94-01, Vol.II, p. 437

[6] Mathewson A,: Proc. Workshop on Vacuum for Future Synchrotron Light Sources, Lure, Orsay, April 1966.

[7] Ushkov V., private communication

[8] Huttel. E., Second Workshop on Vacuum for Future Synchr. Light Sources, Trieste, April 1998

[9] Schulz L., Second Workshop on Vacuum for Future Synchr. Light Sources, Trieste, April 1998