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Alignment and impact angular dependence to O_2 sticking and dissociation on Pt(111) and close-packed steps†

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1 Electronic Supporting information

Table 1 Integrals for the measurements on Pt(111)

H	C_z	C_y	Angle (°)
1891.1	1219.2	-	0
1502.7	830.1	-	0
-	1559	1509.2	0
-	1368.3	1322	0
1685.4	791	-	-30
-	1262.2	1403.3	-30
1621.9	1011.6	-	30
-	848	872.5	30
-	1006.6	1018.8	30
1761.2	1353.8	-	-45
-	1257.8	1491.9	-45
1863.6	1478.8	-	45
1167.4	712.8	-	45
-	660.9	848.3	45
-	495.3	941.7	45

Table 1 shows the integrals of the fit functions of experiments that were performed on Pt(111) at $E_i = 0.33$ eV with varying incident degrees of angular motion. The individually fitted exponents from the experiments were integrated from t_0 of each experiment until the valve closes (around 40×10^3 ms). We find that experiments with the same reaction conditions (E_i, θ_i and the same alteration in H vs C angular motion) do not result in the same integrated sticking probabililies, which would reflect the total adsorbed O_2 in the experiment. For instance, two separate experiments for Pt(111) at 0° incident angle (first two entries in table 1, yield integrals for H that vary by 26% and for C_z by 47%. Hence, the ratio of the integrated signals for H and C_z are also unequal (1.55 vs 1.81). In contrast, the values of S_0 for both alignments match rather well, i.e. 0.178 and 0.173 for H and 0.110 and 0.114 for C_z. The same occurs in entries 12 and 13. For comparison of C_y and C_z, we even find that the integrated values change in opposite direction between two identical experiments (entries 14 and 15). The lack of reproducibility in the (relative) integrals renders us unable to extract coverage dependent sticking probabilities for Pt(111). We find the same lack of reproducibility in the data for the stepped Pt surfaces.

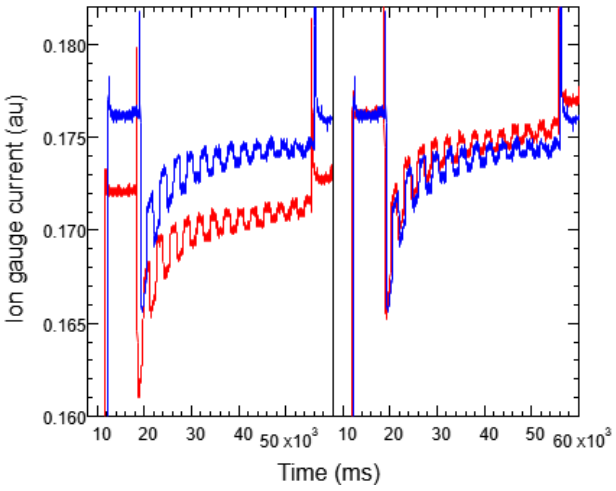

Fig. 1 Initial sticking probability of O_2 as a function of time on a Pt(111) surface for 0.1 eV incident energy for two experiments. The direction of rotational motion of O_2 relative to the Pt surface is switched between H and C_z with the crystal surface at an angle of 0°.

At least one origin of the variation in integrated signals has been identified. Figure 1 shows the traces for the first two experiments on Pt(111), where the direction of rotational motion is switched between H and C_z (entries 1 and 2 in the table). The blue line represents experiment 1 and the red line in experiment 2. In both sections, the data are moved such that the timestamps are the same. In the right panel, the data from experiment 2 is also vertically shifted to match the base ion gauge current prior to the beam's impingement onto the surface. The two experiments are very similar, but the data in experiment 2 relapses to its original ion gauge current after the beam flag is closed, whilst experiment 1 shows a current that does not match the starting current. The fit functions for these experiments are different and result in higher integrals for experiment 1 compared to experiment 2. Possible origins for the non-identical currents prior to and after the experiment have been discussed in the text. One could imagine trying to correct for the appararent time-dependent off sets for each of the two alignments, e.g. by a linear off setting correc-

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tion during the exposure of the crystal to the beam, but a physical basis for this is lacking. This would make the correction, thus, arbitrary.