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Atomic level termination for passivation and functionalisation of silicon surfaces

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Supporting information

Contents:

- **Figure S1**. Effective lifetime versus excess carrier density for TMAH etched silicon without an HF dip, or with HF(2%):HCl(2%) or HF(2%) treatments, with and without an additional superacid-derived passivation treatment.
- **Figure S2**. Effective lifetime versus excess carrier density for treated planar etched silicon without and with an additional superacid-derived passivation treatment.
- **Figure S3**. Effective lifetime at a fixed excess carrier density for treated planar etched silicon before and after a superacid-derived passivation treatment.
- **Figure S4**. Fitted effective lifetime curves for HF(2%):HCl(2%) and HF(2%) treated planar etched silicon without and with an additional superacid-derived passivation treatment.
- **Figure S5.** Fitted effective lifetime curves for HF(50%) treated TMAH etched silicon with different charge densities.
- **Figure S6**. XPS spectra at take-off angle of 90° with respect to the surface parallel for silicon treated with HF(50%) and HF(2%):HCl(2%).
- **Table S1**. XPS elemental composition data for take-off angles of 15° and 90° with respect to the surface parallel for silicon treated with HF(50%) and HF(2%):HCl(2%).
- **Figure S7**. Effective lifetime versus excess carrier density for samples passivated with Al_2O_3 grown by ALD with different chemical pre-treatments.
- **Figure S8**. Si 2*p* XPS spectra at take-off angle of 90° with respect to the surface parallel of an ALD Si_3N_4 coated silicon wafer.

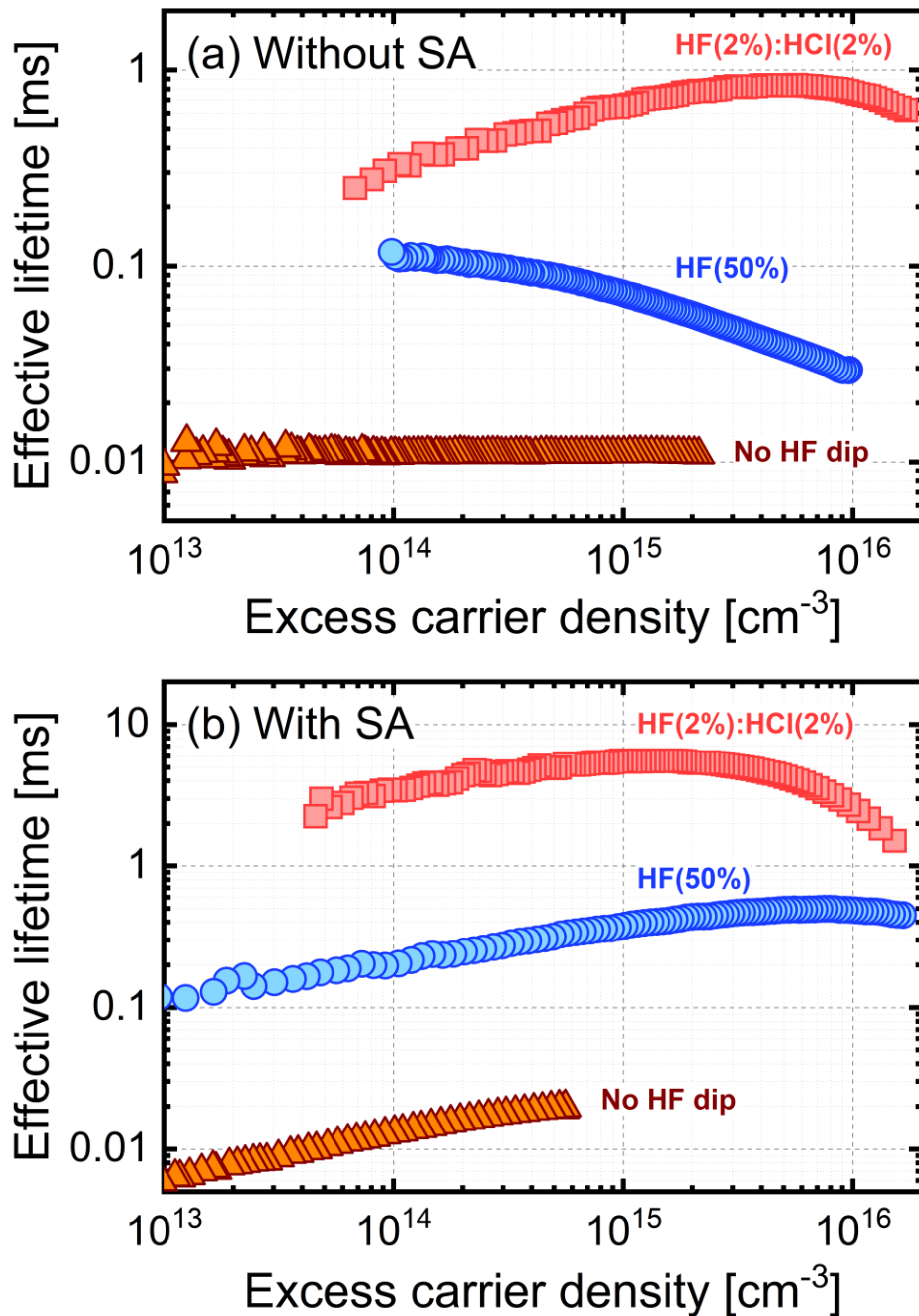

Figure S1. Effective lifetime versus excess carrier density for 700 µm thick 5 Ωcm *n*-type TMAH etched silicon wafers. All samples were first subjected to the same cleaning process (HF dip, SC1 clean, HF dip, SC2 clean), then in (a) samples were subjected to either no HF dip, a 10 min HF(2%):HCl(2%) treatment, or a 10 min HF(50%) treatment. In (b) samples were subjected to the same processes in (a) plus an additional TFSI-pentane superacid treatment.

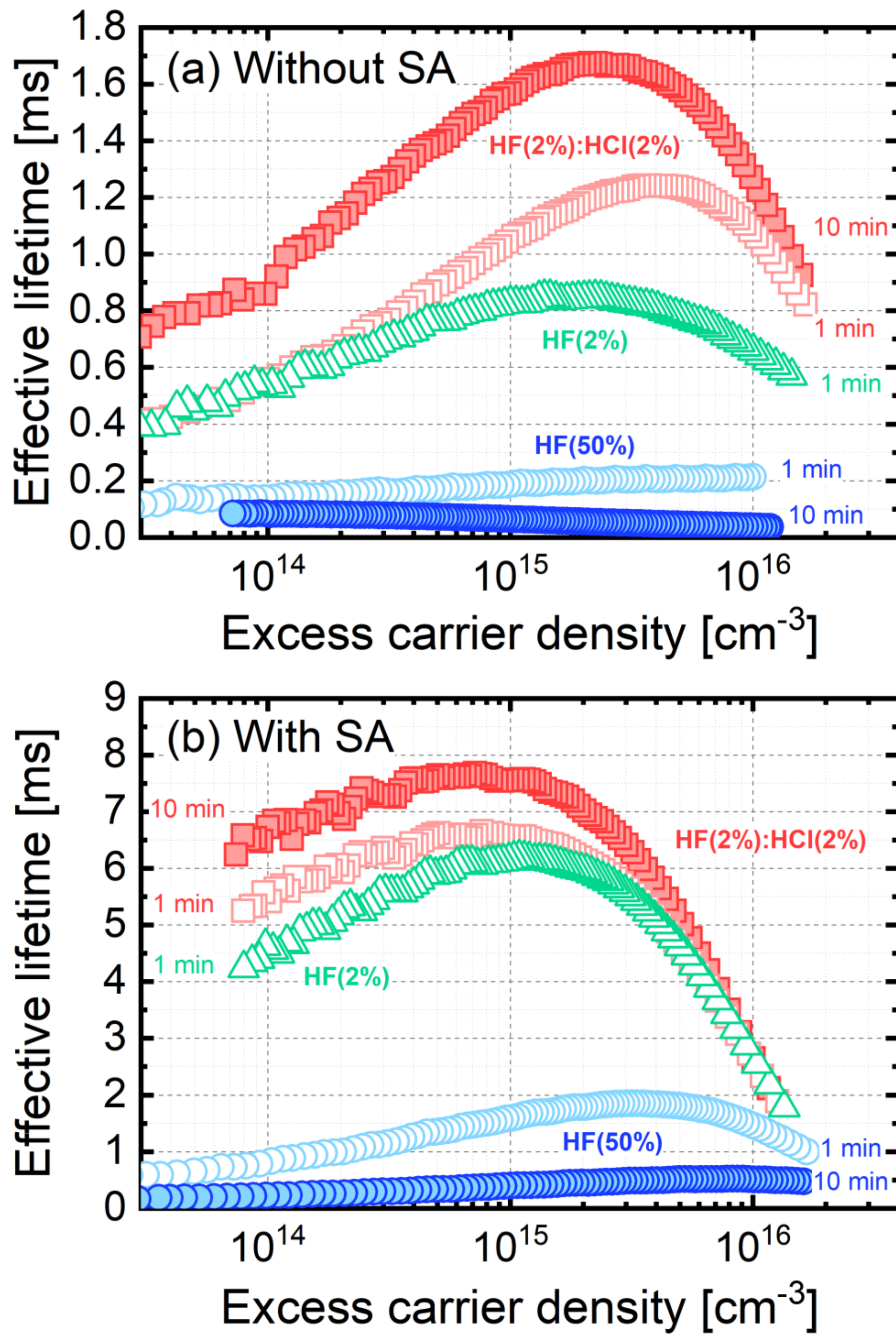

Figure S2. Effective lifetime versus excess carrier density for 700 μm thick 5 Ωcm *n*-type planar etched silicon wafers. In (a) the samples are subjected to HF(2%):HCl(2%), HF(2%) or HF (50%) treatments for the times stated, and in (b) a TFSI-pentane superacid-derived surface passivation scheme (SA) is applied in addition.

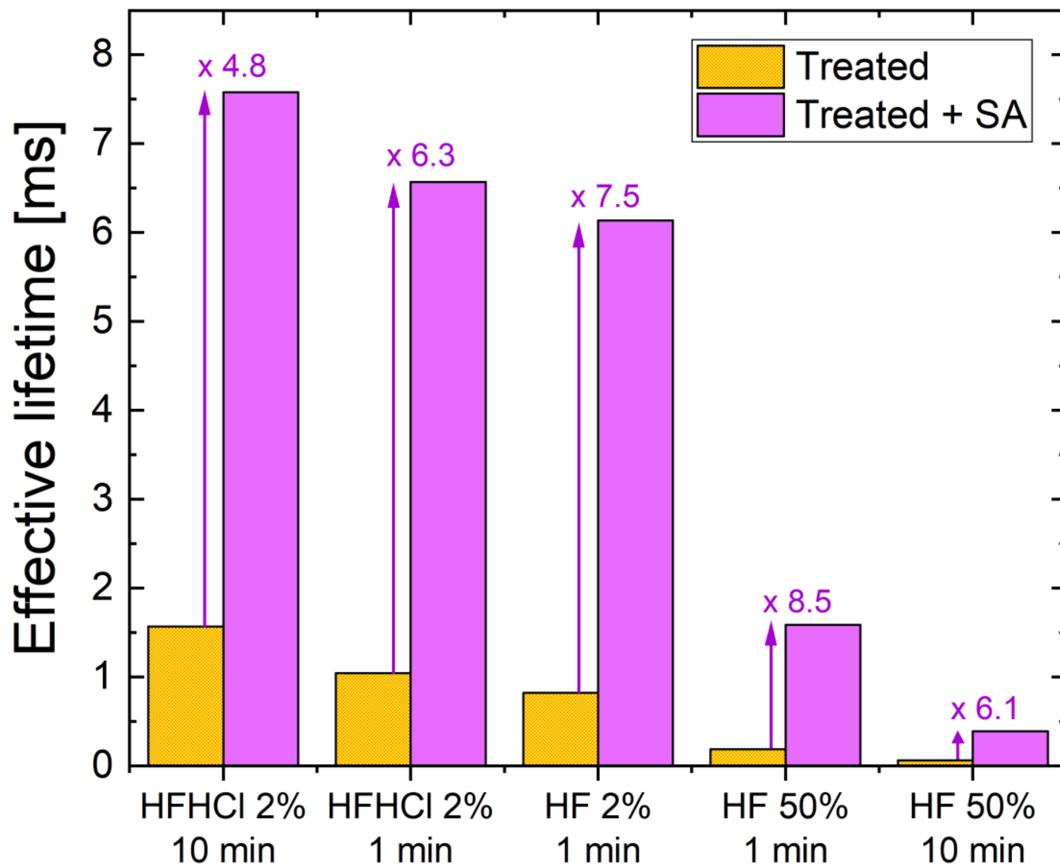

Figure S3. Effective lifetime at an excess carrier density of 10^{15} cm^{-3} for 700 µm thick 5 Ωcm *n*-type planar etched silicon wafers. The left bar of each pair show the effect of the stated treatment only, whereas the right bar shows the effect of the stated treatment plus an additional TFSI-pentane superacid-derived surface passivation scheme (SA). The factor by which the superacid-derived passivation enhances lifetime is also stated.

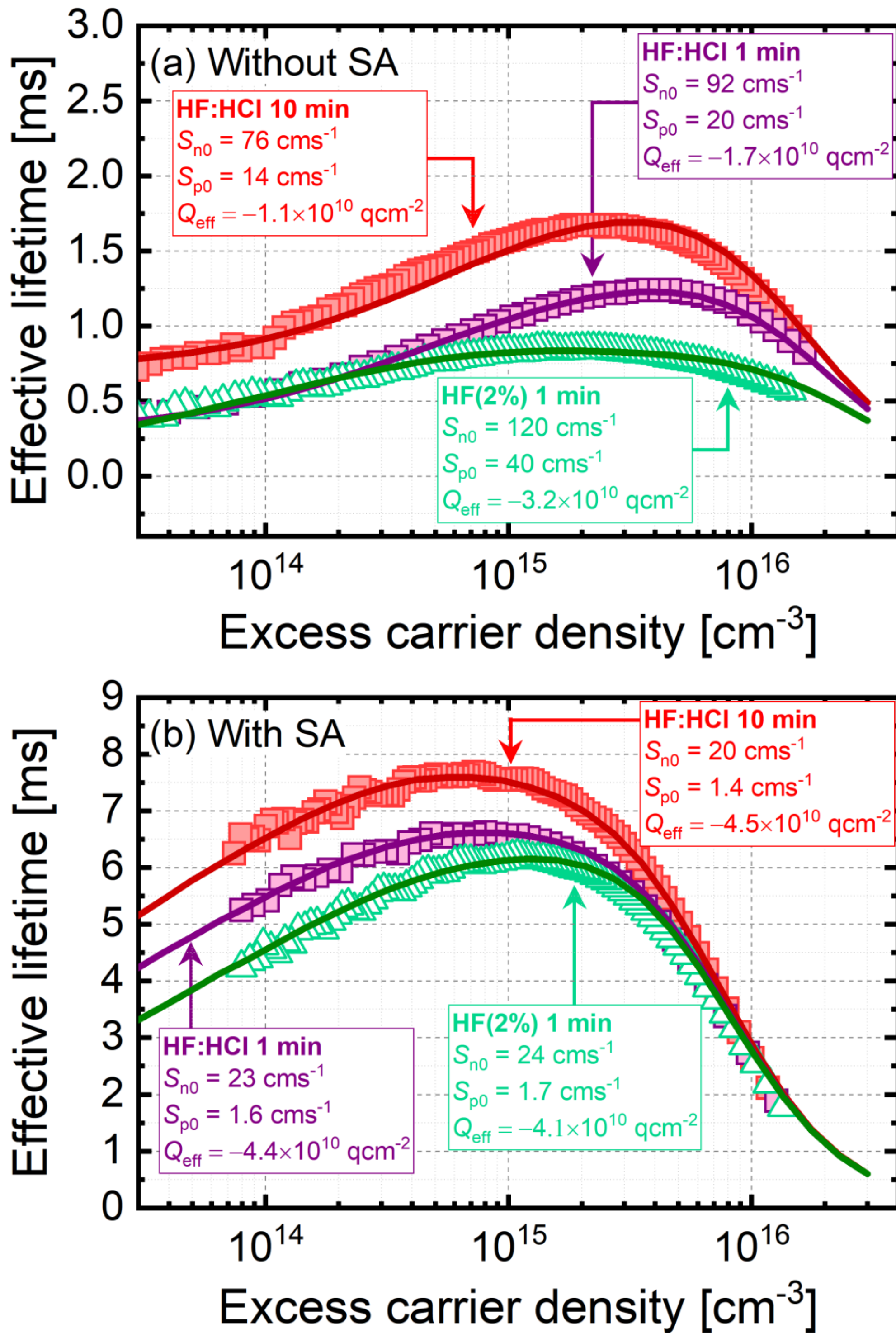

Figure S4. Modelling of effective lifetime as a function of excess carrier density for 700 μm thick 5 Ωcm *n*-type silicon using experimental data for HF(2%):HCl(2%) and HF(2%) treated planar etched silicon in Figure S2. Plot (a) is for samples subjected to just HF(2%):HCl(2%) or HF(2%) treatments, and samples for plot (b) also were subjected to a TFSI-pentane superacid-derived passivation scheme (SA). The parameters used to fit the data are shown in the figure.

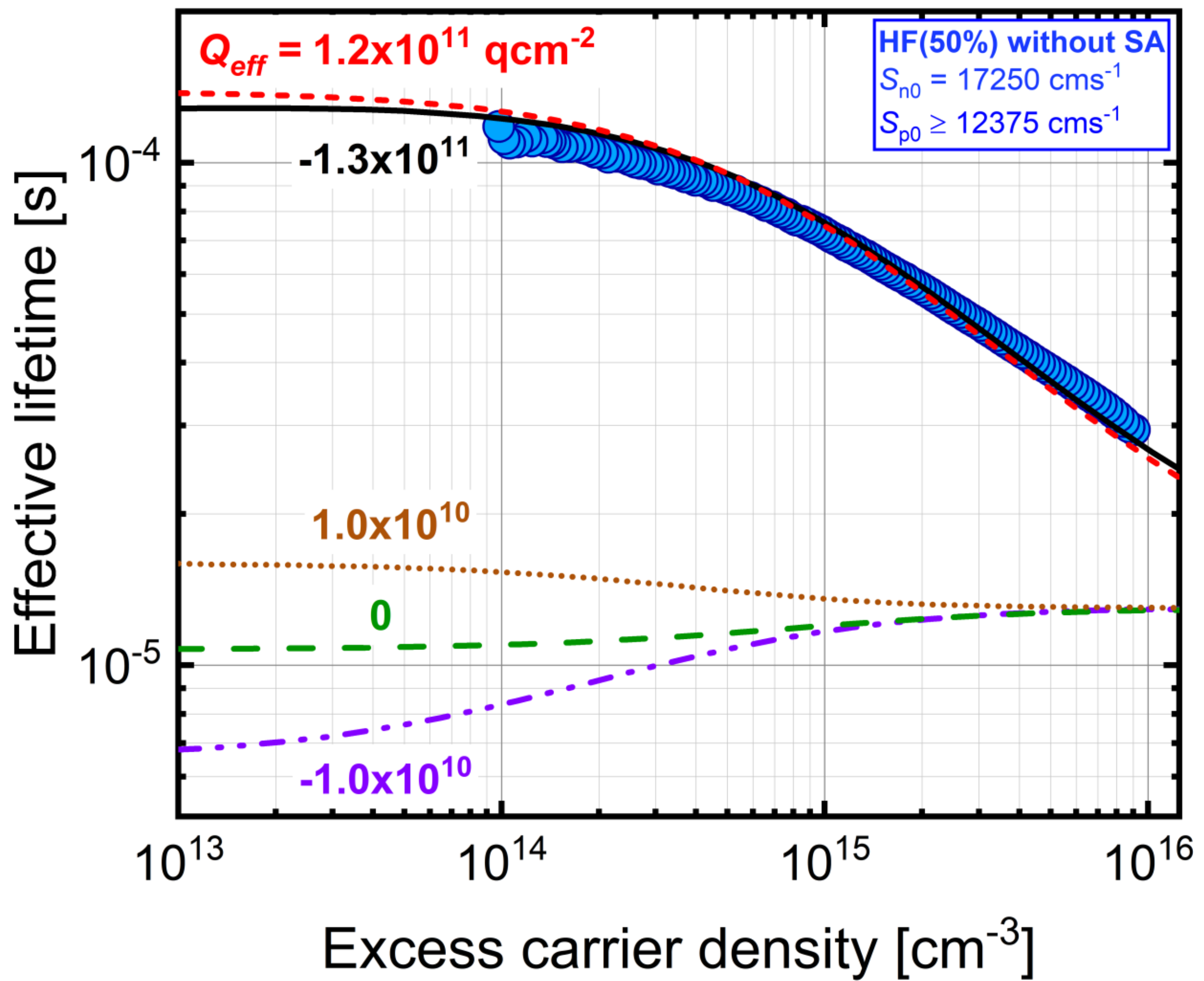

Figure S5. Modelling of effective lifetime as a function of excess carrier density for 700 μm thick 5 Ωcm *n*-type TMAH etched silicon treated with HF (50%) for 10 min (without superacid-derived passivation). The experimental data (blue circles) are from Figure 1 (a). The values of S_{n0} and S_{p0} were fixed, and different values of Q_{eff} were used to generate the curves shown.

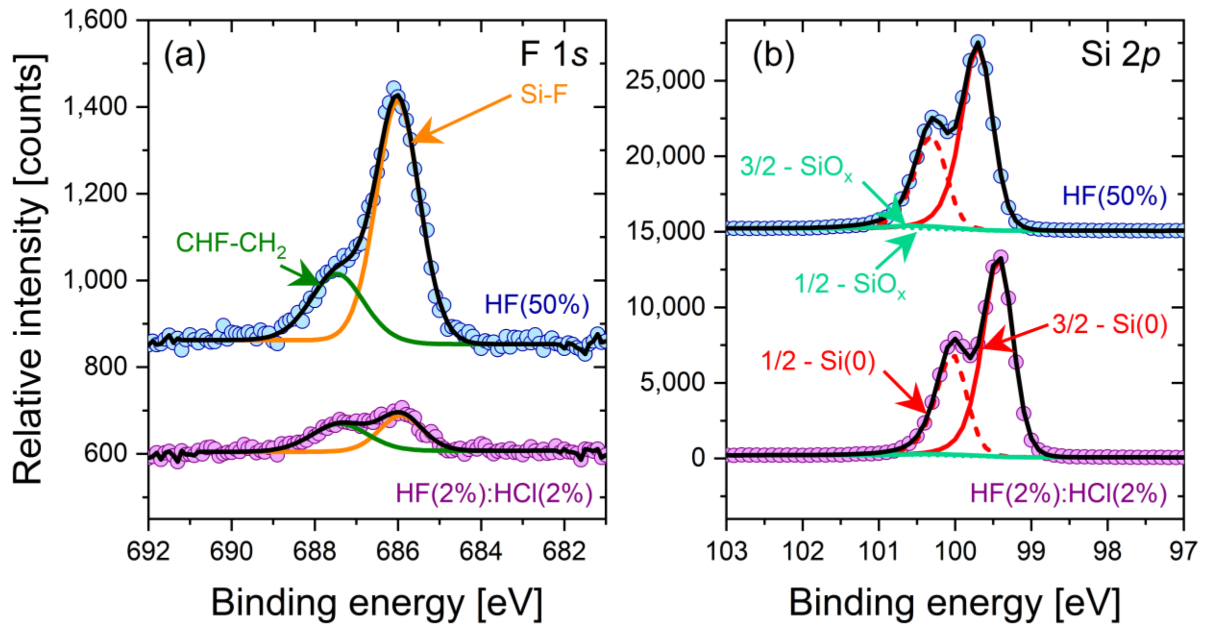

Figure S6. XPS spectra at take-off angle of 90° with respect to the surface parallel for 5 Ωcm *n*-type FZ-Si treated for 10 min with HF(50%) at the top, and HF(2%):HCl(2%) at the bottom. Additional superacid-derived passivation was not applied. Spectra have been offset in the vertical direction for clarity.

Treatment	Take-off angle	Si	C	O	F
HF(50%)	90°	80.77	15.52	1.88	1.84
HF(50%)	15°	53.82	41.33	3.38	1.48
HF(2%):HCl(2%)	90°	83.63	14.14	1.84	0.4
HF(2%):HCl(2%)	15°	50.12	46.08	3.4	0.4

Table S1. XPS elemental composition data for chemically treated silicon surfaces (percentages).

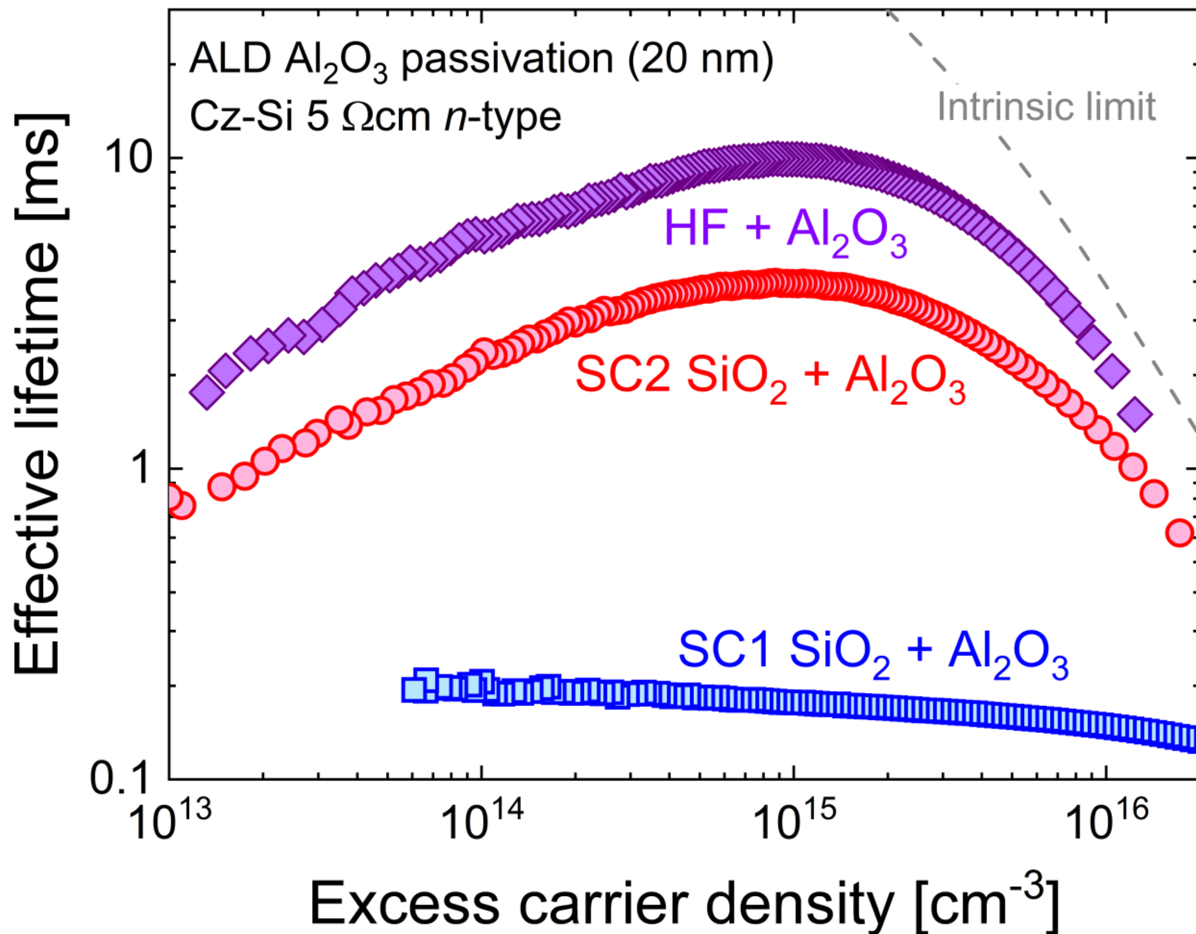

Figure S7. Effective lifetime versus excess carrier density for 130 μm thick 5 Ωcm *n*-type Cz-Si samples from the same wafer passivated with ALD Al_2O_3 after different pre-treatments. The wafer had been alkaline etched (KOH) by the supplier and samples were not subjected to TMAH or planar silicon etching. All samples were initially subjected to the same cleaning process (HF dip, SC1 clean, HF dip, SC2 clean, HF dip). One sample (blue) was then subjected to an additional SC1 cleaning step which grows a thin SiO_2 layer and was not HF dipped prior to deposition. Another sample (red) was then instead subjected to an additional SC2 cleaning which also grows a thin SiO_2 layer and was not HF dipped prior to deposition. The other sample (purple) was HF dipped and pulled dry immediately prior to deposition to remove any oxide formed during cleaning. For all samples, deposition was performed at 200 °C followed by a 30 min 460 °C activation anneal. The intrinsic lifetime limit of Richter *et al.*[1] is also shown. The results demonstrate that the presence of a pre-existing SiO_2 layer results in a lower level of passivation by ALD Al_2O_3.

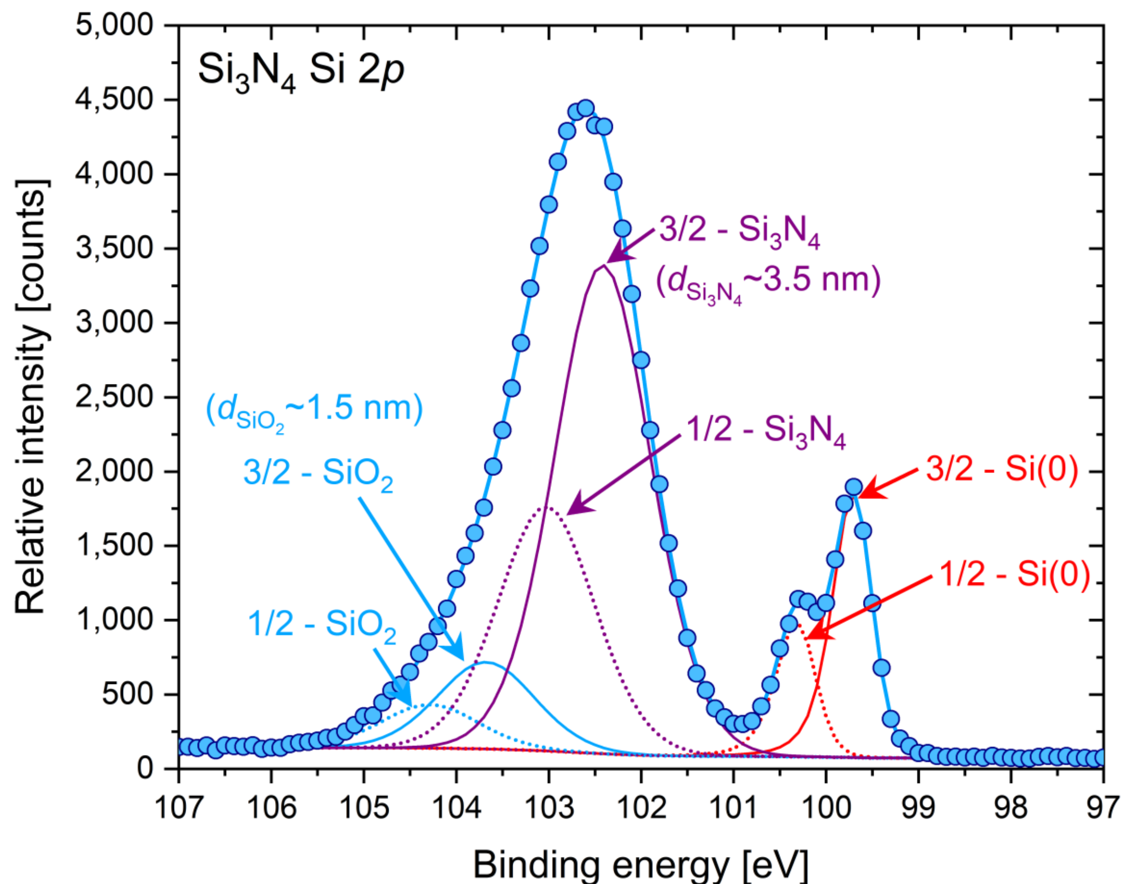

Figure S8. Si 2*p* XPS spectra at take-off angle of 90° with respect to the surface parallel of an ALD Si_3N_4 coated silicon wafer. The solid and dashed lines are fits to the experimental data (blue circles).

Reference for supporting information:

1. A. Richter, S. W. Glunz, F. Werner, J. Schmidt and A. Cuevas, *Physical Review B*, 2012, **86**, 165202