

Supporting Information: Exploring the limits of n-type ultra-shallow junction formation

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Comparison of secondary ion mass spectrometry and pulsed laser atom probe tomography

In the main manuscript we have employed pulsed laser atom probe tomography (PLAPT) for phosphorus depth profiling. In addition, we have obtained secondary ion mass spectrometry mea-

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measurements (Evans Analytical Group LLC) of similarly prepared Si:P δ -doped samples. For both measurements the total integrated phosphorus density agrees well with the active carrier density obtained from low temperature Hall effect measurements ($2.4 \times 10^{14} \text{cm}^{-2}$).

In Figure S1 we directly compare the two measurements, with three main conclusions:

1. The segregation length (equal to the $1/e$ decay length) obtained from the PLAPT data is in good agreement with that obtained from SIMS, as can be seen in Figure S1a.
2. For these abrupt doping profiles, PLAPT provides superior depth resolution to SIMS owing to the lack of ion beam induced artifacts. Recoil-implantation is a well known artifact in SIMS,¹ and manifests here as an artificially broadened trailing edge. This is highlighted in the log-scale plot of Figure S1b.
3. There are no ‘kinks’ in the trailing edge of the phosphorus profile (Figure S1b), validating the use of a Gaussian extrapolation of the PLAPT data.

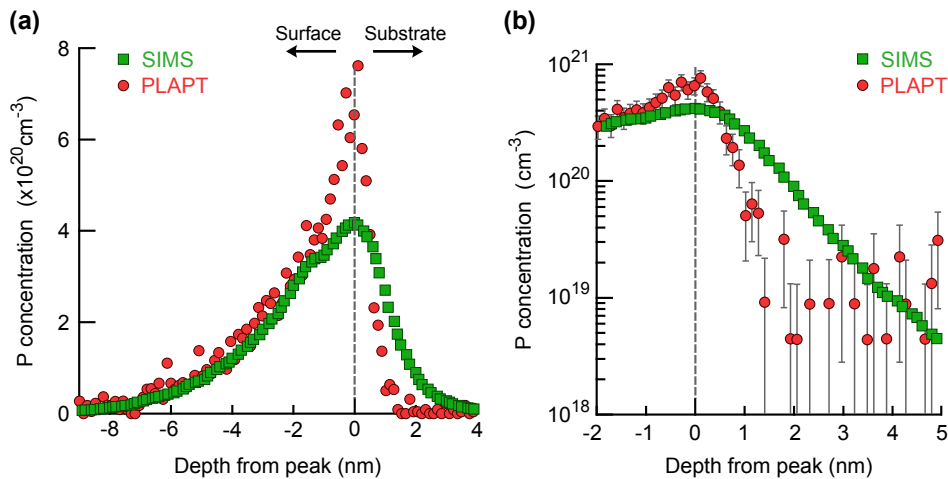


Figure 1: Depth profiling of the physical dopant distribution with SIMS (green squares) and PLAPT (red circles) of two Si:P δ -layers prepared under the same conditions. Both techniques agree on the segregation of the layer (a), but the superior depth resolution of PLAPT is apparent in a rescaled plot (b). The PLAPT data is fitted with an exponential modified Gaussian, which captures an exponential segregation edge and Gaussian diffusion edge..

Data analysis method

The final depth profile is fitted with an exponentially modified Gaussian, describing a Gaussian broadened delta-profile with an exponential segregation edge:

$$N(x) = A \frac{\lambda}{2} \exp \frac{\lambda}{2} (2\mu + \lambda \sigma^2 - 2x) \left[1 - \operatorname{erf} \left(\frac{\mu + \lambda \sigma^2 - x}{\sqrt{2}\sigma} \right) \right] \quad (1)$$

with four fitting parameters: an amplitude A , exponential rate λ , Gaussian central position μ and Gaussian standard deviation σ . When fitting the depth profile, datapoints are weighted by the standard deviation of their binomial error. At low concentrations ($< 1 \times 10^{19}$) each datapoint corresponds to only a few detected phosphorus atoms, and hence has a large uncertainty. The error bars and confidence intervals shown in the manuscript and Figure S1b correspond to 1.96σ .

References

- (1) Baboux, N.; Dupuy, J. C.; Prudon, G.; Holliger, P.; Laugier, F.; Papon, A. M.; Hartmann, J. M. Ultra-Low Energy SIMS Analysis of Boron Deltas in Silicon. *J. Cryst. Growth* **2002**, *245*, 1-8