A practical approach for removing knock-on effects in SIMS depth profiles

Ming Hong Yang, Yupu Li, Charles Hitzman and Robert Odom

Charles Evans and Associates, 301 Chesapeake Drive, Redwood City, CA 94063, USA

INTRODUCTION

Secondary Ion Mass Spectrometry (SIMS) is an effective and powerful analytical technique, widely used in the semiconductor industry, particularly for the development of advanced integrated circuits and devices. One critical application of SIMS is accurately determining dopant concentration profiles (depth profiles) across p-n junctions. As device size shrink, the demand for more accurate depth profiles of shallow junction depths will increase. However, primary ion beam induced mass transport (ion mixing) during SIMS measurements greatly limits the accuracy of p-n junction depth determinations at nanometer depth resolutions because the primary ion beam both displaces and broadens the true depth profile[1-2]. A common yet dramatic illustration of ion mixing effects in SIMS depth profiles is shown in Figure 1 for the case of arsenic and boron implants into Si.

Mass transport phenomena in SIMS produced by the sputtering ion beam can be modeled using linear response theory and true depth profiles can be derived from measured SIMS profiles using deconvolution techniques. To date, several deconvolution algorithms have been developed[3-7] but none of these algorithms have been widely used because the calculations are typically complicated and time consuming. These algorithms also require specific and detailed knowledge of response functions from measurements of delta doped samples which often are not available.

As illustrated in Figure 1, the largest and most important mechanism to ion induced transport in SIMS depth profiles is primary ion knock-on, characterized by an exponential decay of the peak concentration of an implant prepared for delta doped tracer or step functions. The decay length (λ) generally depends on the primary ion beam characteristics (impact energy and incident angle), the tracer element, and the matrix. In this paper, we present a simple deconvolution algorithm developed specifically to remove knock-on contributions to SIMS depth profiles, thereby providing more accurate measurements of junction depths. The results for several specific applications of this approach are presented and a discussion its strengths and limitations is presented.

EXPERIMENTAL

The SIMS response function, $G(x'-x)$, is simply a measured response (concentration) at any given depth, x, to a normalized delta doped tracer at depth, x'. The measured depth profile, $N(x)$, can be expressed as a convolution of the true profile, $N_0(x)$, with a SIMS response function, $G(x'-x)$:

$$N(x) = \int N_0(x')G(x'-x)dx' \qquad (1)$$

The response function for primary ion beam knock-on, $f(x'-x)$, is an exponential decay function which is modeled by:

$$\begin{aligned} f(x'-x) &= 0 && x - x' < -\delta \\ & && (2) \\ f(x'-x) &= \frac{1}{\lambda}\exp\left(-\frac{x-x'+\delta}{\lambda}\right) && x - x' > -\delta \end{aligned}$$

where λ and δ are defined as decay length and depth displacement, respectively. These parameters can be determined experimentally from known delta doped or sharp step profiles. The general response function, $G(x)$, can then be expressed as a convolution of the knock-on response function, $f(x'-x)$, with a different convolution function, $g(t-x)$;

$$G(x'-x) = \int f(t)g(t-(x'-x))dt \tag{3}$$

Differentiating both sides of equation (1) with respect to depth, x, and substituting in equations (2) and (3), we find,

$$\int N_0(x_0)g(x-(x_0-\delta))dx_0 = N(x) + \lambda \frac{\partial}{\partial x} N(x) \tag{4}$$

At the zeroth order of approximation, i.e. assuming $g(t)$ is a delta function, an approximate solution for equation (4) is then given by

$$N_0(x) \approx N(x+\delta) + \lambda \frac{\partial}{\partial x} N(x+\delta) \tag{5}$$

The absolute and relative uncertainties for $N_0(x)$ due to uncertainties in λ can also be easily calculated from equation (5) given by

$$\Delta N_0(x) = \frac{\Delta\lambda}{\lambda} {}^{\partial}\!/_{\partial x} N(x+\delta) \tag{6a}$$

$$\frac{\Delta N_0(x)}{N_0(x)} = \frac{\Delta\lambda}{\lambda} {}^{\partial}\!/_{\partial x} \log(N(x+\delta)) \tag{6b}$$

RESULTS AND DISCUSSION

To verify the validity of the proposed algorithm, we first designed an artificial system to test for self-consistency of the numerical calculations. We then designed several experiments to test the consistency and effectiveness of the algorithm by varying the primary ion impact energies, types of primary ions, and sample configurations. Sources of uncertainties in λ were also evaluated. As shown in Figure 2, an artificial depth profile (Curve a) is created by super-imposing a Gaussian function $[=1e20\exp(-(x-150)^2/400)]$ with random noise. A convolution profile (Curve b) simulating the measured SIMS profile was calculated using equations (1)-(3) with $G(x)=f(x)$, λ = $\delta=40$ Å. The deconvoluted profile (Curve c) was then calculated using equation (5) with the same set of λ and δ values. The results are quite satisfactory and show that this deconvlution method is indeed self-consistent. As expected, the convoluted profile decays exponentially for depths at distance separations greater than twice the full width half maximum (FWHM). The decaying profile can be easily fitted to a straight line on a semi-logarithmic plot with its slope equal to λ. We note that this is a simple and accurate experimental method to determine decay lengths.

In the first analytical experiments, we tested the λ dependence of the algorithm and Figure 3 illustrates the depth profile of a single boron delta layer in silicon using an oxygen primary ion beam and a CAMECA IMS 4f SIMS instrument. Changing the primary beam energy from 3keV to 8keV increases λ from 29 to 50Å. The primary beam incident angles were approximately 52^{o} and 39^{o} to surface normal at 3keV and 8keV, respectively. As described above, λ is determined by fitting the decaying boron concentration to an exponential decay function (dotted lines), $A*\exp(-x/\lambda)+B$. The total sputter depth was determined from crater measurements and the apparent boron peak position was at ~250Å. A boron contamination near the interface (~1300Å) also shows up as a sharp delta function. The displacement, δ, can be calculated directly by subtracting the apparent depth from the known depth. The deconvoluted profiles for 3keV and 8keV profiles using equation (5) are shown as solid lines in Figure 3 for

$\delta = \lambda$. These results show that the algorithm is consistent regardless of the impact energy or λ value. Differences in the rising edges of the deconvoluted profiles are not surprising, since the proposed algorithm does not address forward ion transport processes.

In another experiment, we tested the algorithm on an arsenic doped polysilicon/silicon sample. The arsenic depth profiles shown in Figure 4 were measured with two different primary beam energies using two different instruments. Curve a is the profile produced with a PHI 6650 qaudrupole instrument using a 1 keV Cs^+ beam positioned at a 60^o incident angle and Curve b was acquired with a CAMECA IMS-4f using a 14.5keV Cs^+ primary beam in its standard configuration. Depths were determined from crater measurements. A large knock-on effect is observed for the arsenic profile acquired with a 14.5keV Cs^+ beam as is evident in the slow decay of arsenic concentration. By contrast, knock-on effects for a 1keV Cs^+ beam are significantly less and its arsenic profile was used as a reference for deconvolving the 14.5keV data. The λ value for a 14.5keV Cs^+ beam is 94Å, determined by fitting the decaying portion of the arsenic profile. Using equation (5), the deconvolved profile (Curve c) for the 14.5keV Cs^+ is shown in Figure 3 with δ = 48Å (~0.5λ). Good agreement between the reference and deconvoluted profiles is observed over most of the profile depth. We do observe some disagreement near the arsenic peak which is probably due to matrix effects and deconvolution errors.

In a third evaluation, we tested our algorithm using two Si samples implanted with low energy phosphorus at 2 and 5 keV, respectively. Phosphorus profiles were measured using the PHI 6650 quadrupole instrument with 1keV Cs beam at the incident angle of ~60^o (Curve a in Figure 5), and a CAMECA IMS 4f instrument with a 3keV O_2^+ beam with oxygen flood at the incident angle of ~52^o (Curve b). The phosphorus depth profiles acquired with the PHI 6650 instrument were used as references. As expected, depth profiles acquired with 3keV O_2 beam with oxygen flood exhibit an exponential decay with $\lambda = 31\text{Å}$ for both samples. Using equation (5), the deconvolved profile (Curve c) was calculated and is shown in Figure 5 with δ = 16Å (~ 0.5λ). Good agreement between the reference profile (1keV Cs^+) and the deconvolved phosphorus profiles (3keV O_2^+) was again observed.

These P in Si analyses demonstrate the practical importance of coupling high mass resolution with high depth resolution for optimal SIMS results. Accurate determination of P implants in Si requires the mass resolving power of a double focusing mass spectrometer such as the CAMECA IMS 4f since the mass difference between $^{30}SiH^+$ ions produced from the Si matrix and the $^{31}P^+$ ions is 0.0078 mass units. The mass resolution ($M/\Delta M$) required to separate these two ions is ~4000 which is well beyond the mass resolution of quadrupole SIMS instruments. Unresolved $^{30}SiH^+$ and $^{31}P^+$ ions account for the apparently higher phosphorus concentration detected in the near-surface region in quadrupole SIMS depth profiles of P implants in Si. Furthermore, oxygen flooding using a 3keV O_2 primary beam on the CAMECA instrument reduces surface transient effects, and allows more accurate dose measurements.

We have also evaluated errors due to uncertainties in the estimated λ values. As an example, the absolute and relative error bars for the deconvolved phosphorus profile (2keV) are calculated using equation (6) for $\delta\lambda / \lambda$ = 5%. The overall error for the phosphorus concentration is <10% for the data in Figure 5. The absolute error bars and the deconvolved phosphorus profile are shown in Figure 5.c. The results show that, as expected, the deconvolution is indeed sensitive to the λ value and one must use caution to interpret features if uncertainties in λ are large compared with the deconvolved concentrations. However, in cases where λ is well determined, the calculated profile is a great improvement to the measured profile, particularly when used in conjunction with absolute uncertainty plots for $\delta\lambda / \lambda = 5\%$.

CONCLUSIONS

These results have shown that ion knock-on effects can be effectively removed from selected SIMS profiles using deconvolution methods with simple response functions. This approach also improves the depth resolution of SIMS profiles even when low energy beams are used. Thus, this method should provide improved accuracy in junction depth measurements when knock-on effects significantly alter the true profile shape.

This method is particularly useful for high depth and mass resolution analyses of small areas in which high-energy primary beams are required for good spatial resolution. It can be also used in materials, in which segregation is unavoidable, even if low energy beams are used.

It should also be noted that this deconvolution method depends only on the local depth information and does not require detailed knowledge of the entire profile. Unlike many deconvolution methods developed for SIMS, errors in one part of a profile will not cause errors in other parts unless the separation distance δx is $\leq \lambda$.

References

1) K. Wittmaack, J. Appl. Phys. **53** (1982) 4871.

2) M.G. Dowsett, *Secondary Mass Spectrometry SIMS X*, eds. A. Benninghoven et al., p. 355, John Wiley & Sons, 1995.

3) P.N. Allen, M.G. Dowsett, and R. Collings, Surf. Interface Anal. **20**, 966 (1993).

4) Gautier B. et al., Surf. Interface Anal. **24**, 733 (1996).

5) Gautier B. et al., Surf. Interface Anal. **25**, 464 (1997).

6) M.G. Dowsett and D. P. Chu, *Secondary Mass Spectrometry SIMS XI*, eds. G. Gillen et al., p. 343, John Wiley & Sons, 1997.

7) Gautier B. et al., *Secondary Mass Spectrometry SIMS XI*, eds. G. Gillen et al., p. 347, John Wiley & Sons, 1997.

Figure Captions

Figure 1. Schematic of a p-n junction formed by ion implantation. Thick lines are actual boron and arsenic concentration distributions. The junction is where the arsenic and boron concentrations are equal as indicated. Since the measured arsenic profile (dotted line) is broadened by primary ion knock-on, junction depths determined by SIMS are deeper than true values.

Figure 2. Self-consistency of the proposed deconvolution algorithm demonstrated using an artificial depth profile.

Figure 3. Boron depth profiles and their deconvolution for a boron δ–doped Si sample

Figure 4. An arsenic depth profile and its deconvolution for arsenic doped into a poly-Si on Si material.

Figure 5. Phosphorus depth profiles and their deconvolution for low energy P implants: (a) 2keV, (b) 5keV, and (c) error calculation for (a).

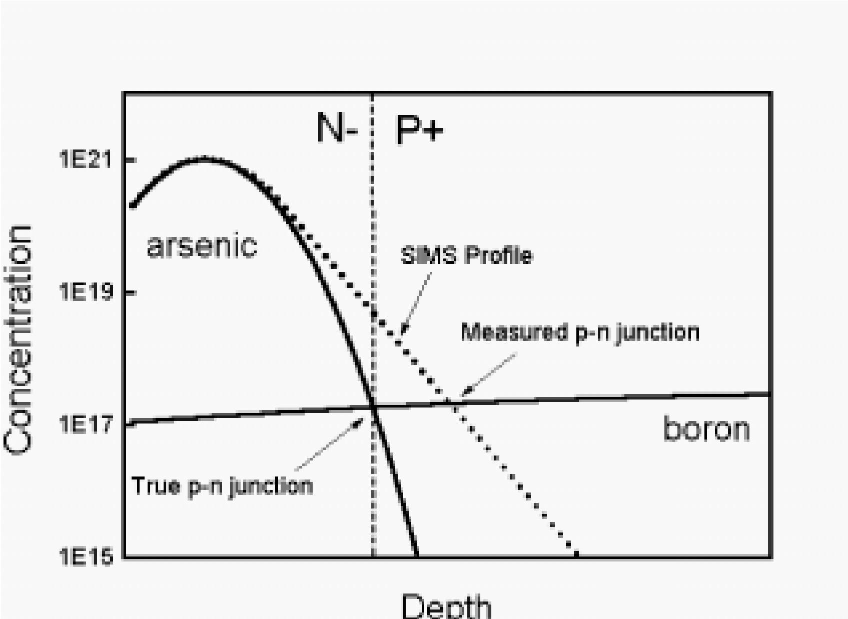

Figure 1: PNJUNC-1.OPJ

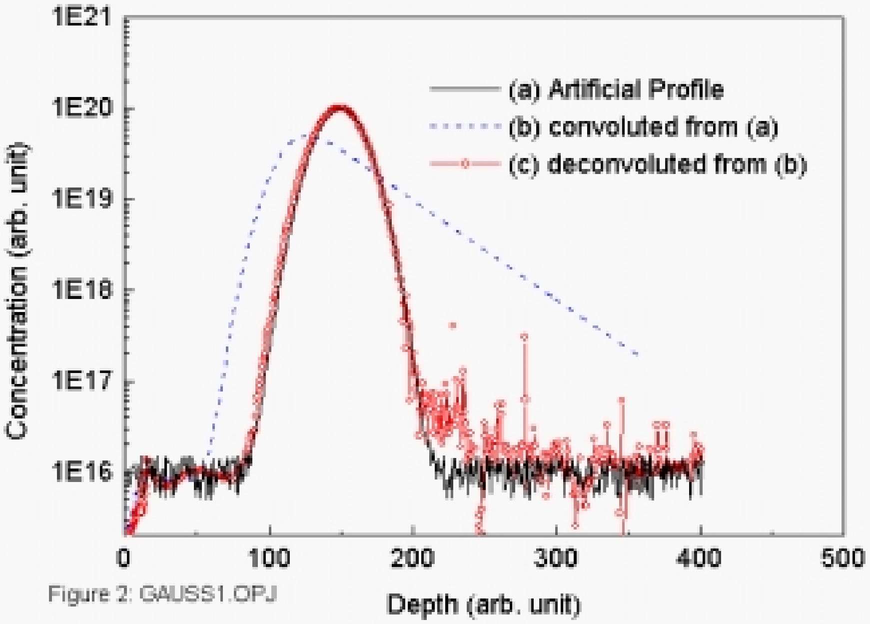

Figure 2: GAUSS1.OPJ

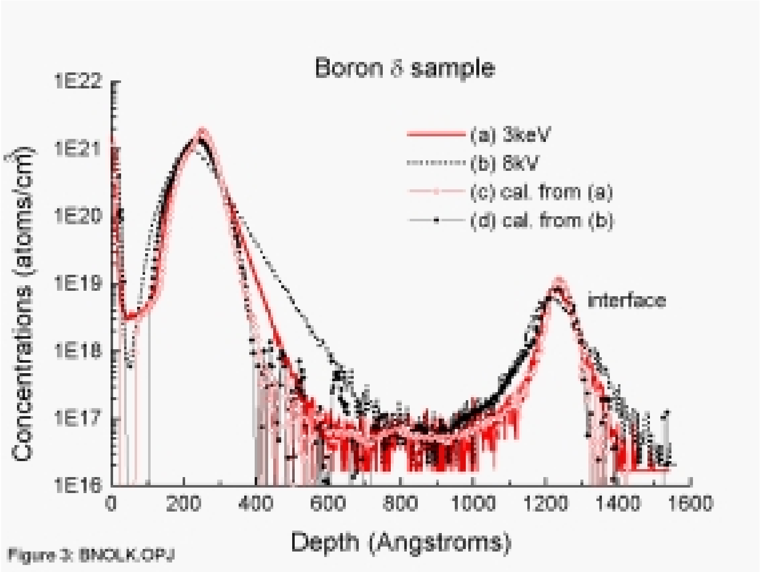

Figure 3: BNOLK.OPJ

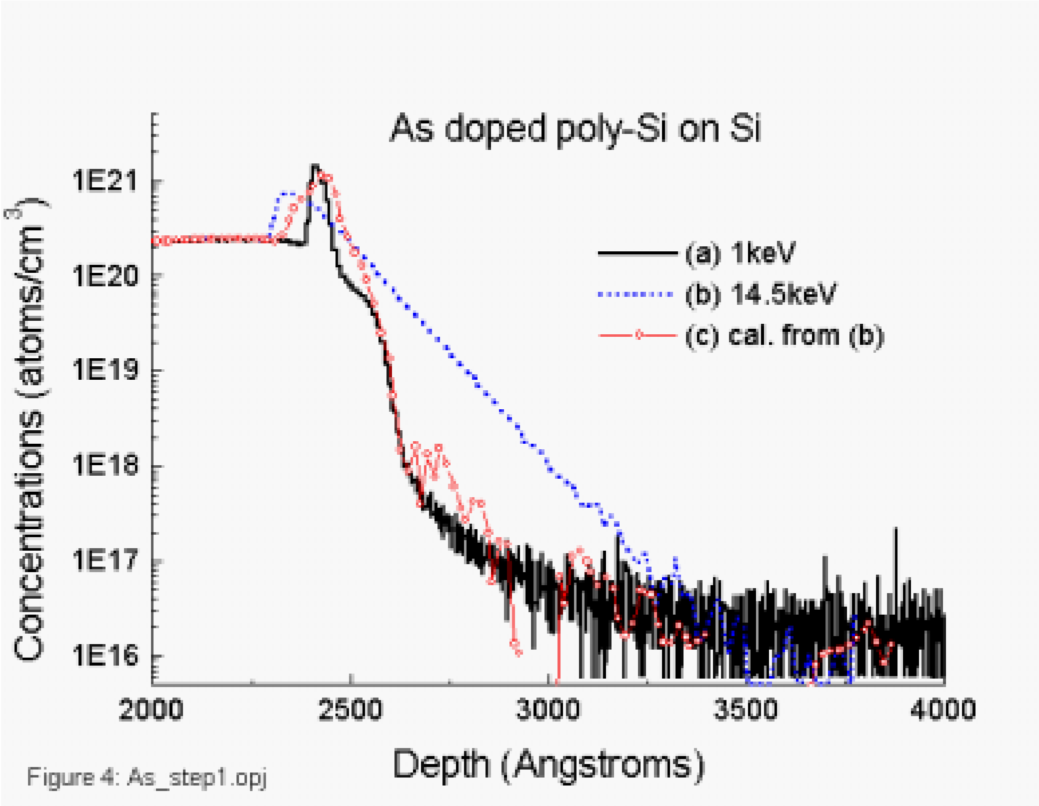

Figure 4: As_step1.opj

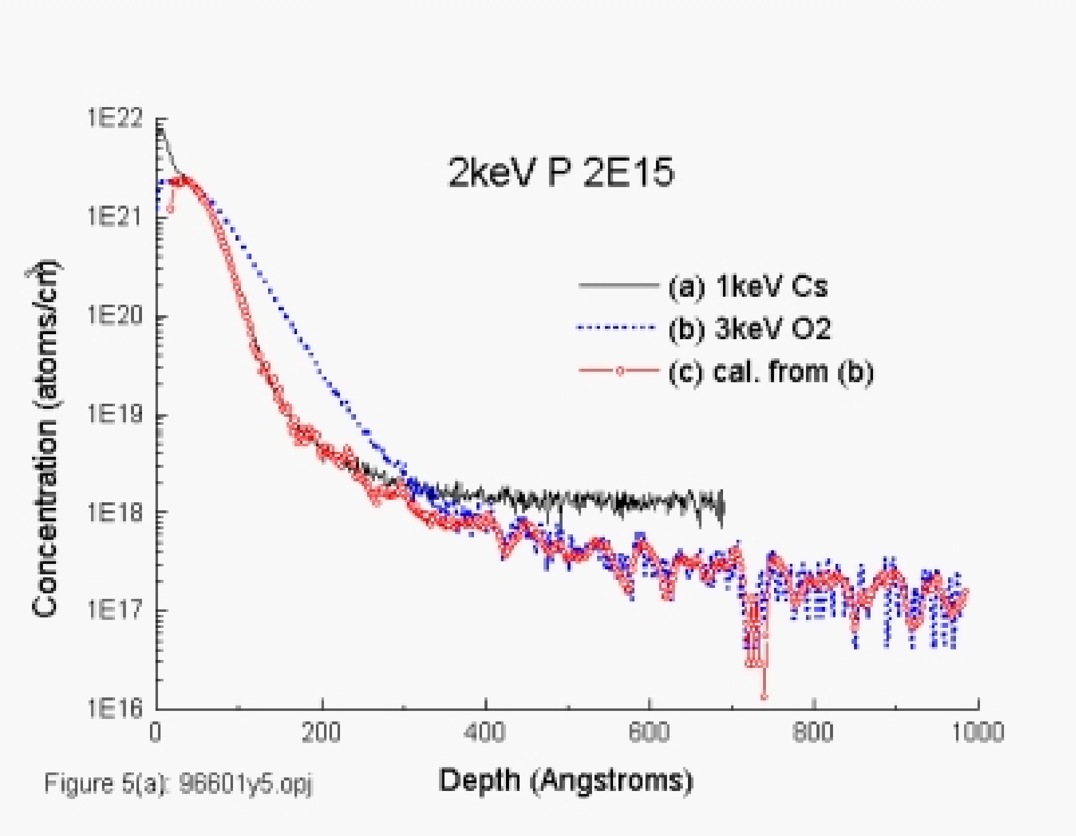

Figure 5(a): 96601y5.opj

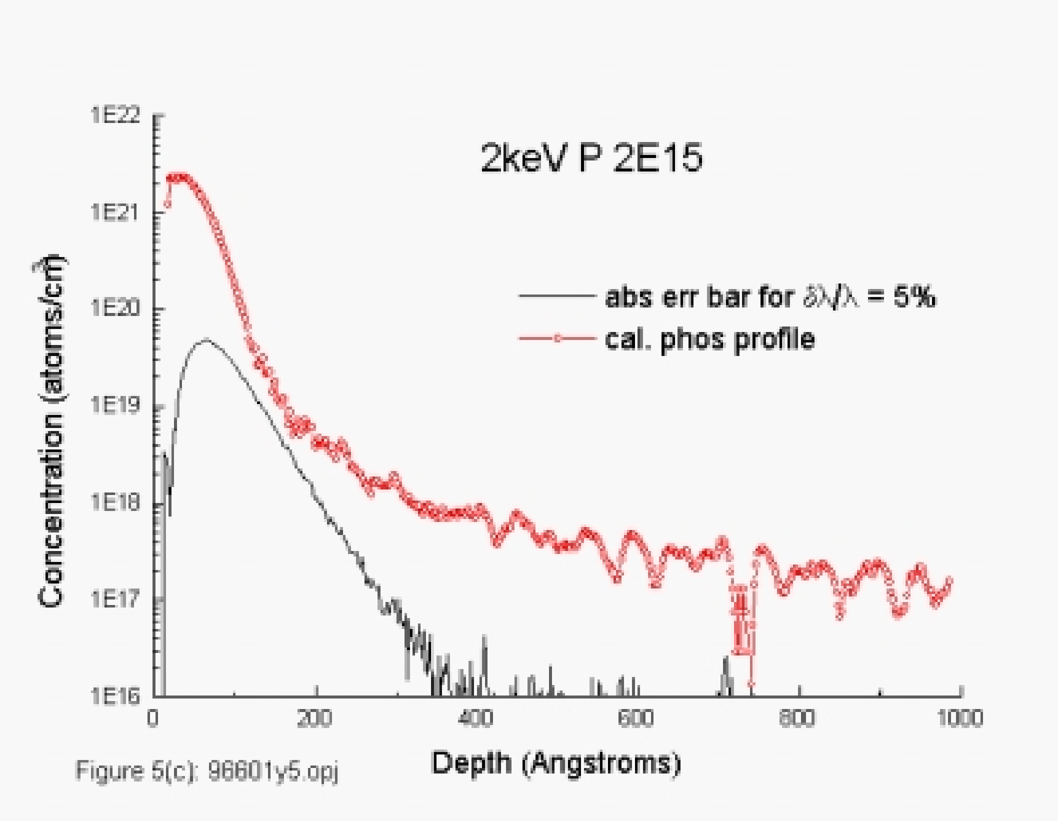

Figure 5(c): 96601y5.opj