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NRL-Contract Monthly Report for February 93

LOW VOLTAGE ELECTRON BEAM LITHOGRAPHY

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The contract has three parts covering aspects of high precision electron beam lithography. (1) Comprehensive computer modeling of the electron beam tool. (2) Experimental determination of the properties of sources, columns, and targets, and (3) The use of silicon single crystals as straightness and orthogonality standards using orientation dependent etching techniques.

Tasks 1-4. Comprehensive modeling of the electron beam tool.

In the last reporting period progress in the calculation of an empirical elastic scattering cross section for electron/atom scattering was reported. This work has now been extended to greater accuracy using a parallel super computer. The code originally based on a PC and needing many days of calculation can now be run in a few minutes. This accurate form of the cross section was sent to Jerry Lowney of NIST, David Joy of Univ. Tennessee, and Cristie Marion of NRL.

The empirical formula are for the scattering cross sections for electron/atom scattering in the range 0.1 to 30keV across the periodic table. The empirical forms are derived from trends in tabulated Mott scattering cross sections (Czyzewski et al.). The form of the total cross section is similar to the previously published cross section (Browning) but has an extra term for the lowest energies and high atomic number. The relativistic correction is now included in the cross section and I have dropped the extra term containing an exponential in the divisor. The total cross section also scales slightly differently with atomic number. It is now (atomic number)^{1.5}. The cross section fit is an engineered fit for fast computation. It was intentional to make all terms in energy simple powers, except one, rather than using what seemed at some times an easier expansion in partial powers. The one exception to this rule is not critical and can be expanded using a Newton-Raphson approach.

The differential cross section is composed of two parts, one part being of the same mathematical form as the screened Rutherford cross section (σ_R), and the second part being an isotropic distribution (σ_I). The screened Rutherford part of the differential cross section is fitted to the half angles of the tabulated Mott differential cross section (the half angle is defined as the angle at which the probability of scattering through an angle into unit solid angle is half that at 0°). The ratio, σ_R/σ_I between the screened Rutherford part of the scattering cross section and the isotropic part of the distribution, is fitted to give the

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same forward to backscattering ratio, (f/b), as the tabulated Mott differential cross sections. This method is the same as suggested in Browning et al.

With empirical forms for the total cross section and the differential cross section a third fit is made to the ratio $\sigma_{\text{Total}}/(f/b)$. Why this ratio? It turns out that the Monte Carlo simulation of backscattering factors is dependent on this ratio. All other things being equal, an increase in the total cross section has an equal and opposite effect to a similar increase in the forward to backscattering ratio. For fitting purposes the $\sigma_{\text{Total}}/(f/b)$ ratio is useful for another reason. Although the total cross section and the differential cross sections are anything but monotonic with atomic number the $\sigma_{\text{Total}}/(f/b)$ ratio is monotonic except at the very lowest energies. This makes it much easier to fit, see figure 1. What is happening is that as the atom size varies periodically with atomic number the density of the atom is also varying, the two effects cancel out as far as the backscattering factors are concerned. This is good news as it justifies our use of monotonically fitted empirical equations in this instance. It is also good news as it means that chemistry, which will change the size of an atom, will not make a first order effect on the electron scattering.

Thus the steps in fitting are: first get provisional forms for the total and the differential cross sections, then adjust the provisional forms to give a better fit to the $\sigma_{\text{Total}}/(f/b)$ ratio and then simplify them to remove redundant parameters. Using these adjusted forms the backscattering coefficients for normal incidence are calculated. The equations are then fitted to the backscattering coefficients calculated directly from the Mott cross sections. Straightforward expressions for the cross sections was found to give the backscattering results covering all the major trends with energy and atomic number and within a few percent accuracy for the backscattering coefficient. This has now been tested from Be to Au for 0.1 to 30keV. The results are shown graphically for Al, Cu and Au in figure 2. There are 100,000 trajectories per point in the fit.

For the total cross section the fit is based on the total cross section previously published (Browning). This fit is in essence the same form as the screened Rutherford cross section plus some terms for the low energy high atomic number end. The exponential part of the divisor has been removed because of the computational overhead. There are now only three terms in energy, one linear term, a square root term and an inverse square root term, again this was done for computational speed but it works quite well. The total cross section does not require a relativistic correction. The two term dependence on Z that was previously published has disappeared as it was easier to fit two parameters in the Monte Carlo simulation than three.

The final equation is:

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$$\sigma_{\text{Total}} = \frac{5.0 \times 10^{-18} Z^{1.5}}{(E + 0.015Z^{1.33}E^{0.5} + 0.00035Z^2 / E^{0.5})} \text{ cm}^2$$

Although it might seem surprising it turns out that the half angle for the differential scattering distribution is nearly constant over the entire periodic table. I think this is because the low angle forward scattering is dependent on the size of the atom not the size of the nucleus. Atom sizes are pretty well constant across the periodic table except where different electron shells are filled or half filled. It is in the half angles however that I have most misgivings as it is here that the results of Reimer and Lodding and Czyzewski et al (Hartree Fock) seem to diverge most. For example at 1keV for carbon Reimer and Lodding have a half angle of 10° and Czyzewski of 6.8°. This disagreement is worse in other places. I imagine that this difference is due the differences in the atomic model but I am disturbed that this should be the case as the forward scattering angle is rather important for many applications. The half angles also show some of the largest variations with atomic number for example, the half width for He is 8° and Li 5°. My fit ignores all the variations due to shell sizes, and I've decided to let it ignore all changes with Z, which are smaller than the variations due to the input assumptions. The average half widths for low atomic numbers are 7° and is a minimum at higher atomic numbers at around 5°. The average is 6° which implies a Rutherford screening parameter for all Z of:

$$\alpha = 7.0 \times 10^{-3} / E$$

Where E is the electron energy.

The screening parameter is only used to define the distribution of the scattering from the Rutherford part of the differential cross section and has no meaning with respect to the total cross section. The scattering angle for the Rutherford part is defined by:

$$\cos(\theta) = 1 - \frac{2\alpha R}{1 + \alpha - R}$$

Where R is a random number between 0-1. The scattering angle for the isotropic distribution is:

$$\cos(\theta) = 1 - 2R$$

After fixing the screening parameter a critical part of the process is then to get the forward to backscattering ratio correct.

The forward to backscatter ratio is defined as:

$$\left(\frac{F}{B}\right) = \frac{\int_0^{90} \sin \theta \cdot d\sigma / d\Omega \cdot d\theta}{180 \int_0^{90} \sin \theta \cdot d\sigma / d\Omega \cdot d\theta}$$

The forward to backscatter ratio for the screened Rutherford part of the differential cross section is proportional to $(1+1/\alpha)$. The (f/b) ratio from the tabulated Mott data was fitted by adding in the extra backscattering effects using the isotropic distribution. With no other fitting this gave quite a good result in the Monte Carlo calculations.

With the two parts of the equation for the parameter $\sigma_{\text{Total}}/(f/b)$ the fits were adjusted to give a smaller number of terms and round numbers. But care was taken not to change the individual cross sections too much so as to become unphysical. The fit to this ratio at energies above 5keV is in Z^2 (and monotonic) which is identical to that expected from the screened Rutherford cross section. With a very simple equation for the relative areas of the screened Rutherford cross section to the isotropic it was found that most of the trends in the Monte Carlo results obtained by Czyzewski et al were reproduced.

The final stage in the fitting process was to use Monte Carlo simulation and 50 data points taken from Czyzewski et al and from Reimer "Scanning electron microscopy" page 136 to fine tune the fitting parameters. The fitting used a constrained parameter mean square fit procedure and 10000 trajectories per data point. (a major computing effort). After tidying up the least significant figures the ratio of Rutherford to Isotropic areas is:

$$\frac{\sigma_{\text{Rutherford}}}{\sigma_{\text{Isotropic}}} = \frac{300E^{1-Z/1000}}{Z} + \frac{Z^3}{3 \times 10^5 E}$$

I used the same modified Bethe energy loss equation as Czyzewski et al This is David Joy's fix to the Bethe equation:

$$\frac{dE}{ds} = -785 \frac{\rho Z}{AE} \ln\left(\frac{1.166(E+U)}{J}\right) \text{eV/A}$$

Where $t=0.85$

As can be seen from figure 2. which shows the comparison of the empirical fit (solid lines) with Czyzeski's and Reimers's data (symbols) the fit for Al, Cu and Au is pretty good. Figure 3 shows the fit for C and Ag added, these aren't so good, but the fit for Be is good (not shown as only two data points) The fit for Ag is poorest in the knee at low energy, which bucks the trends set by Cu and Au, this could be corrected by changing the $E^{0.5}$ terms in the total cross section. The fit for C is high but as the fit at 10keV and 30keV for Be is very good I did not want to force the fit down. The knee for Au is too high in the fit and the knee for Al is too low so the fit does have some warts. However, as these results have similarly sized deviations as the use of different atomic models it seems hardly worthwhile to increase the number of decimal points in the fit.

I tried very hard not to have fractional powers but one was unavoidable. I've attached a description of a method to treat the power term $E^{1-Z/1000}$. This uses a modification of the Newton-Raphson algorithm to follow the power with small changes in energy and is much faster than a call to a full precision routine.

Refs.

- R.Browning, Appl.Phys.Lett 58, p2845 (91)
- R.Browning et al. J.V.S.T (B) 9, p3578 (91)
- Z.Czyzewski et al. J.Appl.Phys. 68, p3066 (90)
- L.Reimer and B.Lodding, Scanning 6, p128 (84)
- D.C.Joy and S.Luo, Scanning 11, p176 (89)

Anticipated Work in the next reporting period.

Feedback from Jerry Lowney of NIST shows some differences between his results and Stanford's these differences need to be resolved.

Further exposures of the Si metrology pattern will be made and the standards mounted on a carrier.

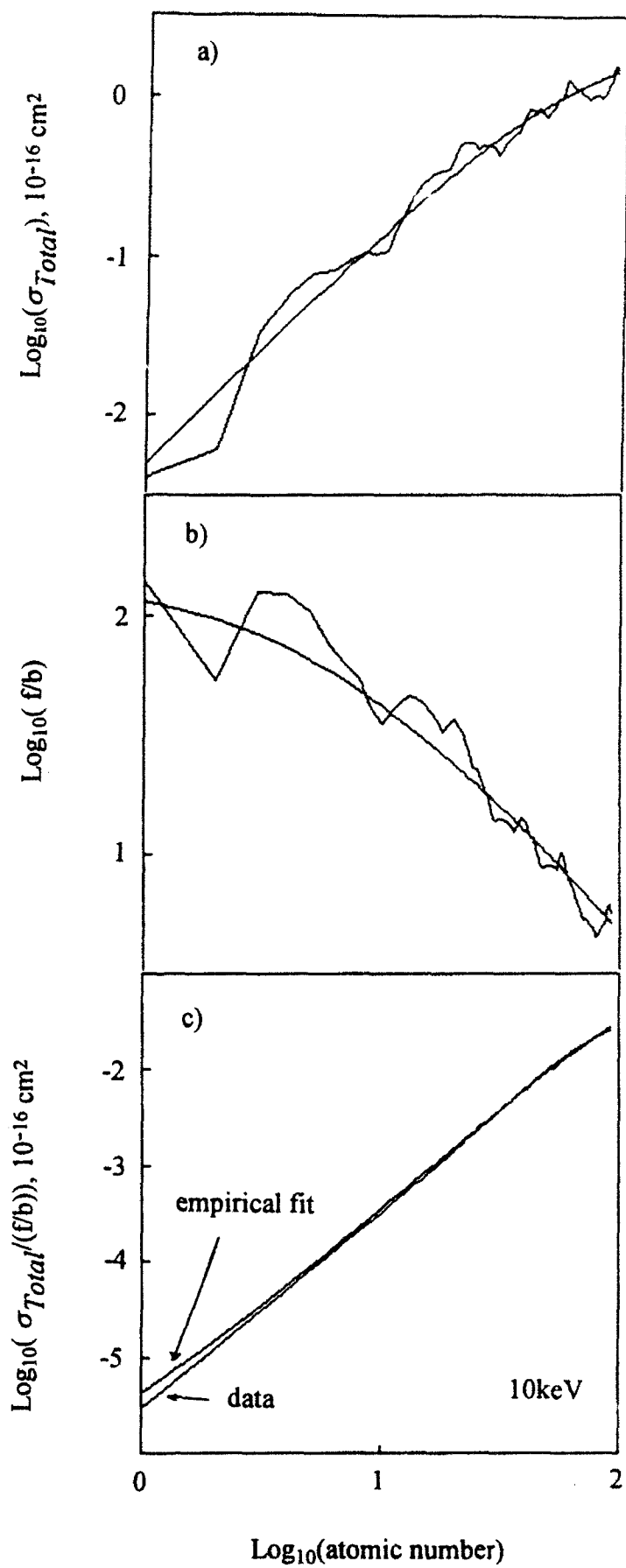


FIG 1

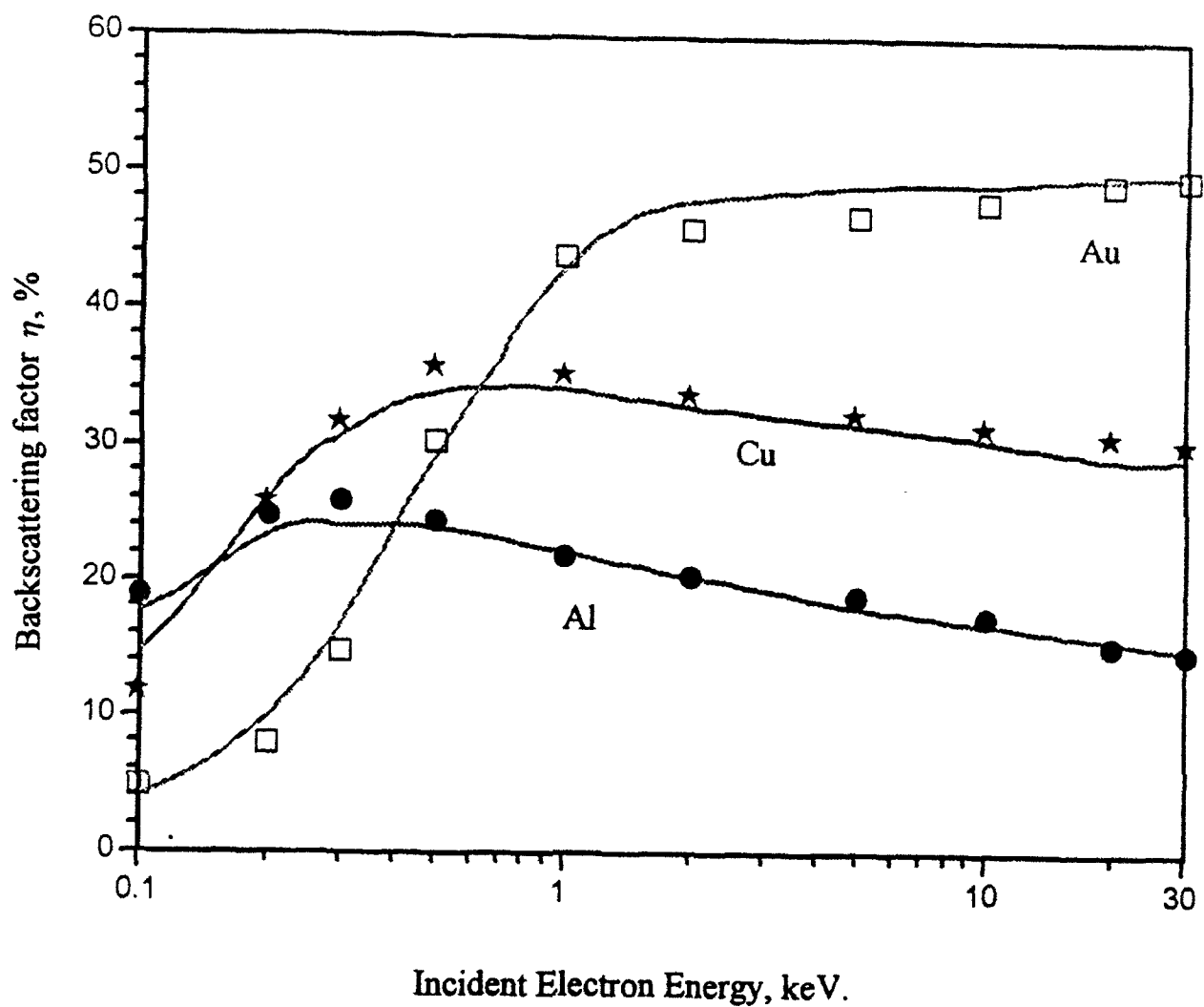


FIG 2.

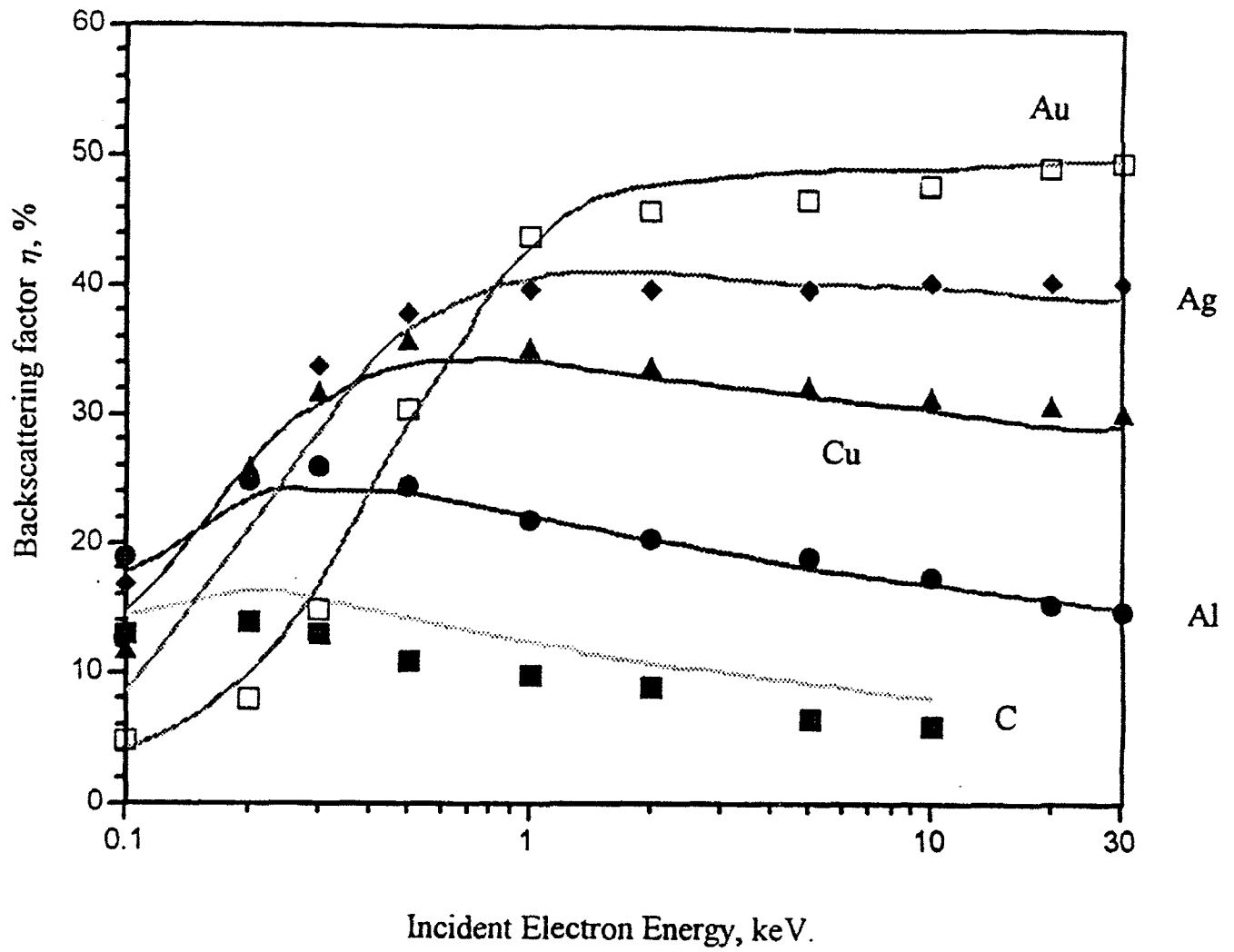


FIG 3 .

An Iterative Method for Generating Fractional Powers.

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Abstract

A simple and accurate iterative method is presented to follow fractional powers during slowly varying parametric changes. The method is based on the Newton-Raphson method for calculating roots but does not require a calculation of the inverse power term. Thus the method can be used for irrational powers.

A common requirement in finite element computer simulations of physical processes is to calculate fractional powers at each temporal or spatial step. The computation overhead to calculate these fractional powers is heavy and under some circumstances can dominate the calculation time. This is particularly true when using empirical equations which have fitted parameters and powers. However, in many cases fractional powers do not need to be calculated to the full precision available and an approximation could be made. It is also the case that in physical simulations that the parameters need to be slowly varying, so as to be considered continuous. One method for calculating roots is the Newton-Raphson method. This method is simple and accurate and reaches high precision after a few iterations, the speed of convergence depending on the initial guess. Only one iteration can make a significant increase in precision if the initial guess is close. These observations suggest that the Newton-Raphson method could be adapted to follow fractional powers of a slowly varying parameter.

The Newton-Raphson method for calculating fractional roots uses a successive approximation from an initial estimate. The method derives the root, z , for:

$$z = x^y \quad (1)$$

where y is a fractional power and:

$$y = 1/p \quad (2)$$

where p is an integer. An initial estimate z_0 is made. Then the first iteration uses the formula:

$$z_1 = 1/p [z_0 (p-1) + x / z_0^{(p-1)}] \quad (3)$$

to provide a new estimate z_1 . The method works for p an integer or a rational number but not for irrational numbers because the last term would contain an irrational power and this

is the same problem as finding an irrational root. We need to modify the method to avoid this problem.

Our method starts by knowing accurately the value of z_0 given an initial parameter value x_0 . With our first result known to high precision we can write by definition:

$$z_0^{(p-1)} = x_0 / z_0 \quad (4)$$

If we change x_0 to $x_0 + \Delta x = x_1$ and then substitute x_1 for x in equation 2 then we have:

$$z_1 = 1/p [z_0^{(p-1)} + (x_0 + \Delta x) z_0 / x_0] \quad (5)$$

where z_1 is the $1/p$ th root of x_1 . Thus our estimate is the previously calculated fractional power and we are no longer required to calculate the fractional power in the last term of Newton's method. Therefore the power can be integer, rational or irrational.

Expanding equation (5) for fractional powers between $y = 0$ to 1 shows us that the error in the limit of small step size is maximum at $y = 0.5$ and proportional to the square of the step size. This observation means that we can correct for the first order error. If we choose a step size $\Delta x/2$ then for one step we have a quarter of the error and for two steps we have half the error of a step size of Δx . Then we have:

$$z_I \text{ (one step } \Delta x) = T + e \quad (6)$$

and

$$z_{II} \text{ (two steps } \Delta x/2) = T + e/2 \quad (7)$$

where T is the true value and e is the error for one step Δx .

The first order error can thus be removed as

$$T = 2z_I - z_{II} \quad (8)$$

The results of using equation 5 without error correction for following $x^{0.5}$ as the parameter x decays from 100 to 0.1 in 66 steps of $-0.1x$ are an error per step of 1.5 parts in 10^3 and an accumulated error of 1 part in 10. If first order error correction is used the error per step is 1.5 parts in 10^6 and an accumulated error of 1 part in 10^4 . The accumulated error is linear in step size and the error per step decreases as the square of the step size. For $x^{0.95}$ the accumulated error for the uncorrected algorithm is 2 parts in 100, this is sufficient accuracy for the $E^{(1-z/1000)}$ term in the Monte-Carlo equation.