Ion Channeling Revisited

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B. L. Doyle and P. Rossi

Radiation Solid Interactions Department 01111
Sandia National Laboratories
Albuquerque, NM, USA

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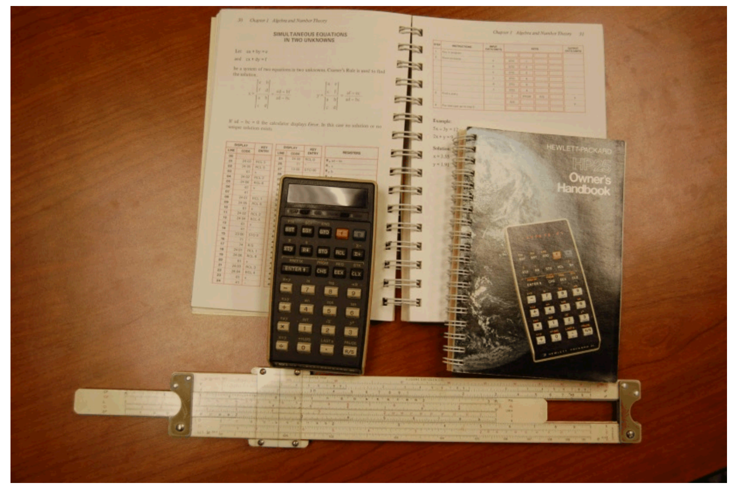
Why revisit channeling?

- The three IBA Handbooks have been an extremely useful references to practitioners of IBA.

- However, because they first came out (1977) when powerful desk top computers were unavailable, many of the calculations involved (and still require) manual interpolation from tables and readings from graphs. This was particularly true for the chapters on Ion Channeling written by Appleton and Foti [4], Swanson [5], and Swanson and Shao [6].



- This paper describes an Excel program that makes it easy to calculate axial and planar channeling half angles and minimum yields for any ion, of any energy on virtually all mono-elemental bcc, fcc and diamond lattice crystals or polycrystals.

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LAB NEWS

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This & That

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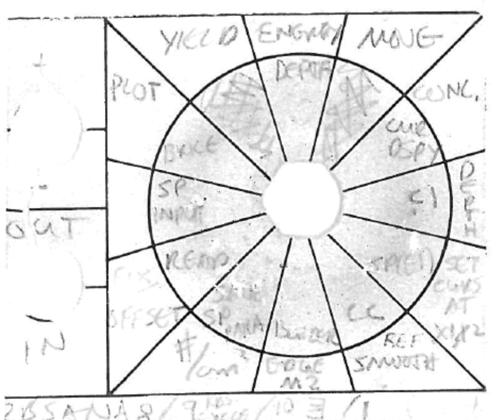
Barney and the Beast – On the Milepost page (page 10) is a 15-year service anniversary photo of Barney Doyle (1111) pictured "mind-melding" with the 15-year-old PDP-11/34 computer that his organization still uses. It's one of the oldest computers around the Labs that's still in service, Barney says, and maybe the very oldest. Sandians?

MILEPOSTS

LAB NEWS

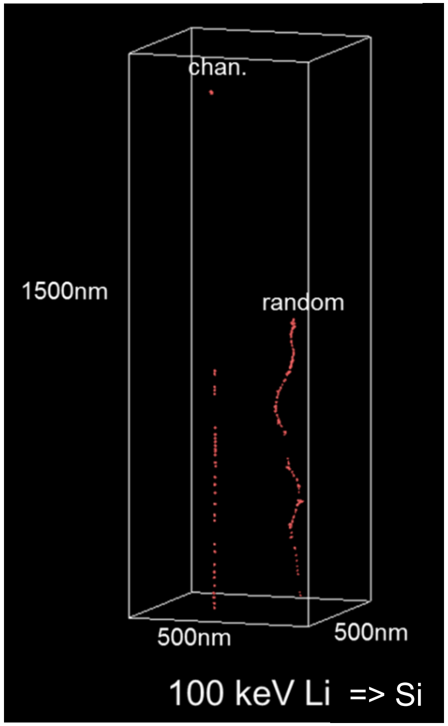
November 1992



Barney Doyle
1111

Why revisit channeling? (2)

- There has been a resurgence of interest in ion channeling.
- From the standpoint of ion beam analysis (IBA)
  - Use of backscattering and IBIC of finely focused and scanned low energy ions
    - from a He-Ion Microscope (HIM) V. Veligura, G. Hlawacek, R. van Gastel, H.J.W. Zandvliet and B. Poelsema, Beilstein Journal of Nanotechnology, Vol. 3 (2012) 501.
    - and 100 keV Li Channeling to get straight trajectories in IBIC experiments to image single collision cascades at Sandia
- From the standpoint of radiation effects R&D
  - Effect of unintentional channeling of ions used to simulate neutron induced displacement damage
    - El-Atwani, Osman, A. Suslova, T.J. Novakowski, K. Hattar, M. Efe, S.S. Harilal, and A. Hassanein, "In-situ TEM/heavy ion irradiation on ultrafine- and nanocrystalline-grained tungsten: Effect of 3 MeV Si, Cu, and W ions" Mater Charact (2014), 99 (2015): 68-76.
    - and single crystals of GaAs photovoltaic devices at Sandia
  - If the ions accidentally channel, less displacement damage will result as compared to the case where they do not channel.
  - It is therefore important to know and quantify how this grain-by-grain disparate generation of damage can affect mechanical properties.



Axial Channeling

3.1.1 Axial $\psi_{1/2}$ half-angles

The specular or characteristic axial channeling angle ψ_1 is calculated using the formula given in Lindhard's famous paper [10]:

$$\psi_1 = \sqrt{\frac{2Z_1Z_2e^2}{Ed}}\ (radians)\ , \qquad (3.1)$$

Where Z_1 and E are the atomic number and Energy (MeV) of the projectile. Z_2 is the atomic number of the target atom, e is the fundamental electron charge which equals $1.44\text{x}10^{-5}$ MeV-Å and *d* is the separation of the atoms in Å along the axial direction <uvw>.

$$d = f_a\, cc \qquad (3.2)$$

cc is the conventional cell size and

$$f_a = \frac{\sqrt{u^2+v^2+w^2}}{1+N}\ , \qquad (3.3)$$

where *N* is the number of atoms between and along the same direction as <uvw>. In general, *N=0* except *N=1* when uvw are all odd with no zeros for bcc, uvw have two indexes odd and one even including zero for fcc, and uvw are all odd or have two indexes odd and one even including zero for diamond lattices.

The quantity u_1 represents the vibrational amplitude of the atoms perpendicular to the axis and is expressed as:

$$u_1 = 12.1\left(\left(\frac{\phi_D(x")}{x"}+0.25\right)\left(\frac{1}{M_2\theta_D}\right)\right)^{1/2}\ (Å), \qquad (3.4)$$

Where θ_D is the Debye temperature, M_2 is the target atom mass in amu. Both of these values are also obtained after Z_2 is entered in the program using a lookup table, and

$$x" = \frac{\theta_D}{T}\ . \qquad (3.5)$$

$\phi_D(x")$ is the Debye function.

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Debye Function

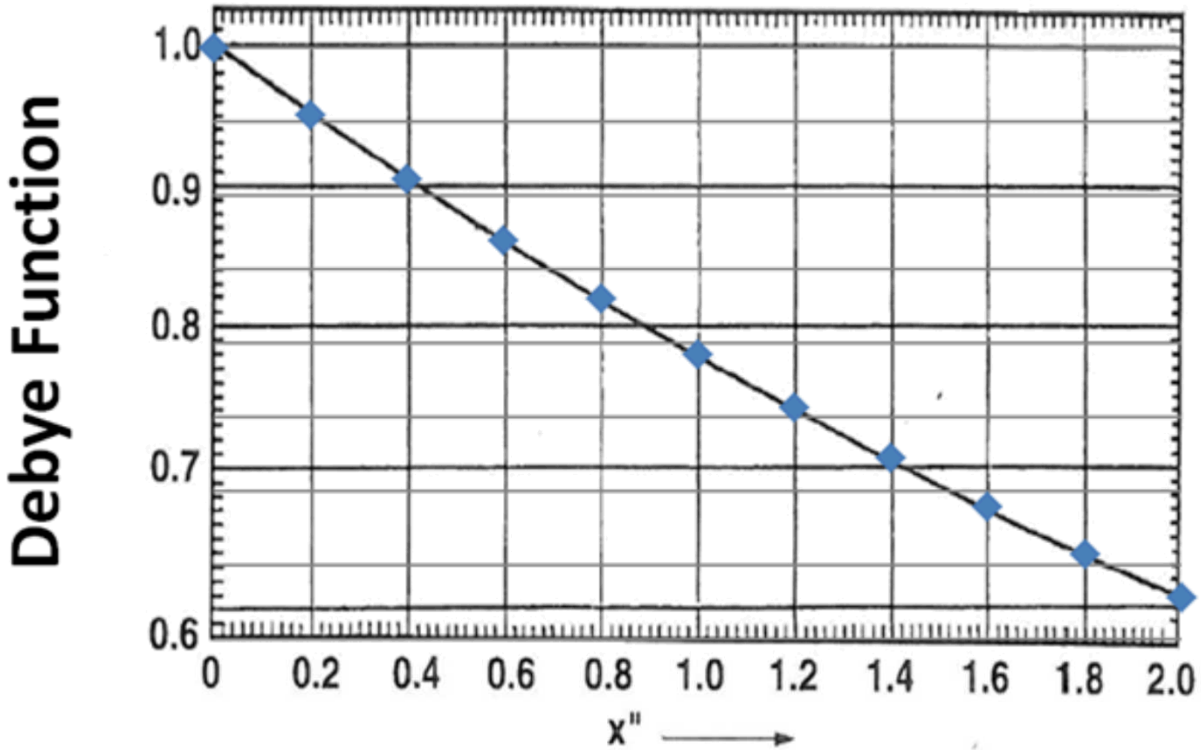

Figure 1 Parameterized Debye Function

$$\phi_D(x'') = \exp(-x''/4.3) \qquad (3.6)$$

Channeling ½ angle and adimentional string function

A parameter x' relates the vibration amplitude to the Thomas-Fermi screening length, a in the equation:

$$x' = 1.2\frac{u_1}{a} \qquad (3.7)$$

Several different expressions for a can be found in the Handbooks, but as will be discussed later, the one that provided the best agreement with the channeling data listed in the Handbooks was that of Firsov [11]:

$$a = 0.04685 / (Z_1^{2/3} + Z_2^{2/3})^{1/2} \qquad (3.8)$$

The expression for the axial $\psi_{1/2}$ half angles given in [5] is:

$$\psi_{1/2} = 0.8F_{RS}(x')\psi_1 \text{ for } \psi_1(rad) < \frac{a}{d} \qquad (3.9)$$

$$\psi_{1/2} = 7.57\sqrt{\frac{a\psi_1}{d}} \text{ for } \psi_1(rad) > \frac{a}{d} \qquad (3.10)$$

Where F_{RS} is the square root of the adimensional string potential using Moliere's screening function and calculated using Monte Carlo techniques by Barrett [12]. The parameterized fit to the F_{RS} function plotted in A15.2 in [5] is shown in Fig. 2.

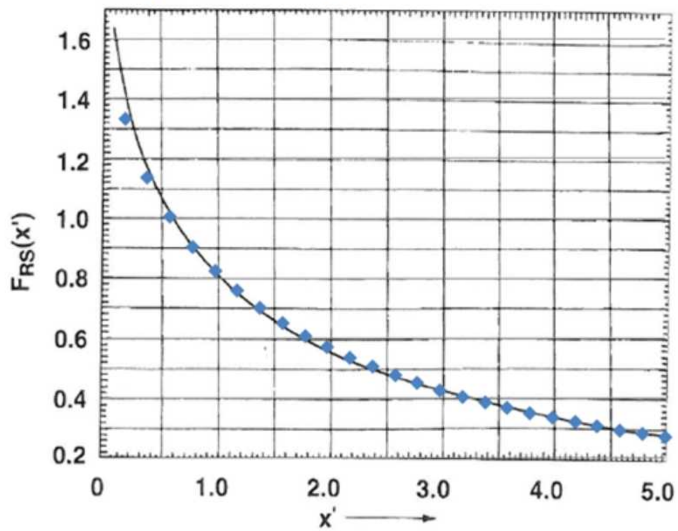

Figure 2 Parameterization of the F_{RS} adimensional function for axial channeling

$$F_{RS} = 1.9\exp(-x'^{0.53}/1.2) \qquad (3.11)$$

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axial χ-min

3.1.2 Axial χ_{min} minimum yield/dechanneling probability

In this report we are equating the χ_{min} minimum yield equations found in [5], which are usually associated with Rutherford Backscattering channeling spectra, with the probability that ions perfectly aligned to axial directions do not actually channel. This is because instead of being aimed into the open space between rows of atoms, they hit the top surface atoms of this row.

Two equations are given in [5] for the axial χ_{min}. The first is attributed to Lindhard [10]:

$$\chi_h^{<uvw>} = Nd\pi(2u_1^2 + a^2) \, , \tag{3.12}$$

and the second to Barrett [12] which is:

$$\chi_h^{<uvw>} = 18.8Ndu_1^2\sqrt{1+\frac{1}{\xi^2}} \, , \tag{3.13}$$

where

$$\xi = 126\frac{u_1}{(\psi_{1/2}d)} \tag{3.14}$$

We have selected the second form given by Barrett to use in the program.

Overlayers

3.1.3 Effect of amorphous overlayers on axial channeling

According to Lugujjo and Mayer, the reduction of the $\psi_{1/2}$ half-angle due to small angle scattering due to the presence of amorphous overlayers is:

$$\theta_c = \frac{a_{13} E \psi_{1/2}}{\left(2Z_1 Z_3 e^2\right)}, \quad (3.15)$$

$$\chi_{min} = P(\theta_c), \quad (3.16)$$

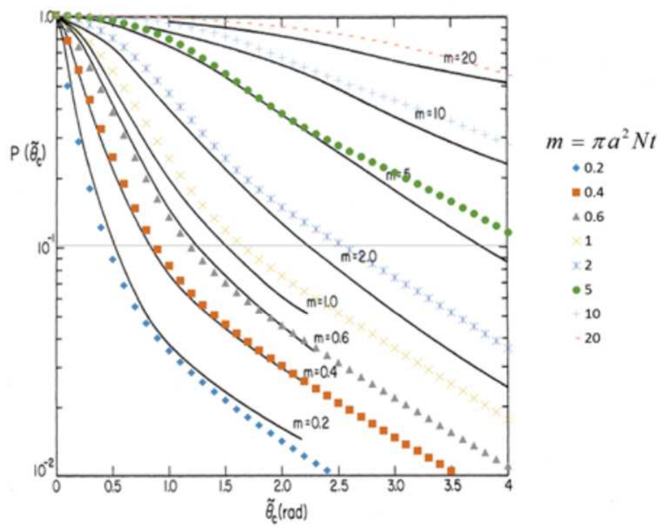

Figure 3 P function describing dechanneling due to amorphous overlayers together with the parameterization presented here.

In this parameterization the overlayer thickness parameter m is given by

$$m = \pi a^2 N t \quad (3.17)$$

Where a is the Thomas-Fermi screening distance given in Equation 3.15, N is the concentration of overlayer atoms per $Å^3$ and t is the thickness in $Å$

$$P = 0.92\exp(-\theta_c^{p_c}/c) + 0.08\exp(-\theta_c^{p_b}/b) \quad (3.18)$$

$$p_c = 0.974 m^{0.288} \text{ and } c = 1.17 m^{0.41} + 0.16 m^{1.8} \quad (3.19)$$

$$p_b = 1.646 m^{0.372} \text{ and } b = 0.44 m^{0.64} + 0.048 m^{2.32} \quad (3.20)$$

Planar Channeling

3.2.1 Planar $\psi_{1/2}$ half-angles

The expression for planar $\psi_{1/2}$ half-angles is given in [5] as:

$$\psi_{1/2}^{p} = 0.72 F_{PS}(x', y')\psi_a \,, \tag{3.21}$$

where

$$\psi_a = \sqrt{\frac{2Z_1Z_2e^2}{Ed_p}}\ (radians)\,. \tag{3.22}$$

N is the concentration of target atoms in units of $\#/\AA^3$ and d_R is the atomic separation of the planes ($\AA$) for the usual [hkl] Miller index orientations.

$$d_p = f_p cc \tag{3.23}$$

Where cc is the size of the conventional cell.

For bcc lattices, this factor is:

$$f_p^{bcc} = \frac{1}{\sqrt{h^2+k^2+l^2}} \text{ for } h+k+l = even\,,\ \text{ or } f_p^{bcc} = \frac{1}{2\sqrt{h^2+k^2+l^2}} \text{ for } h+k+l = odd\,. \tag{3.25}$$

For fcc lattices, this factor becomes:

$$f_p^{fcc} = \frac{1}{\sqrt{h^2+k^2+l^2}} \text{ for } h,k,l \text{ all odd}\,,\ \text{or } f_p^{fcc} = \frac{1}{2\sqrt{h^2+k^2+l^2}} \text{ for } h,k,l = \text{ not all odd}\,. \tag{3.27}$$

For diamond lattices, the factor is:

$$f_p^{fcc} = \frac{1}{2\sqrt{h^2+k^2+l^2}} \text{ for all } h,k,l \text{ or } f_p^{fcc} = \frac{1}{4} \text{ for all permutations of [001]} \tag{3.29}$$

FPS(x',y') in equation 3.21 is the square root of the adimensional planar potential using Moliere's screening function and also calculated using Monte Carlo techniques by Barrett [12].

$$x' = 1.6\left(\frac{u_1}{a}\right),\ \text{and} \tag{3.30}$$

$$y' = \frac{d_p}{a} \tag{3.31}$$

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planar ½ angle and adimentional planar function

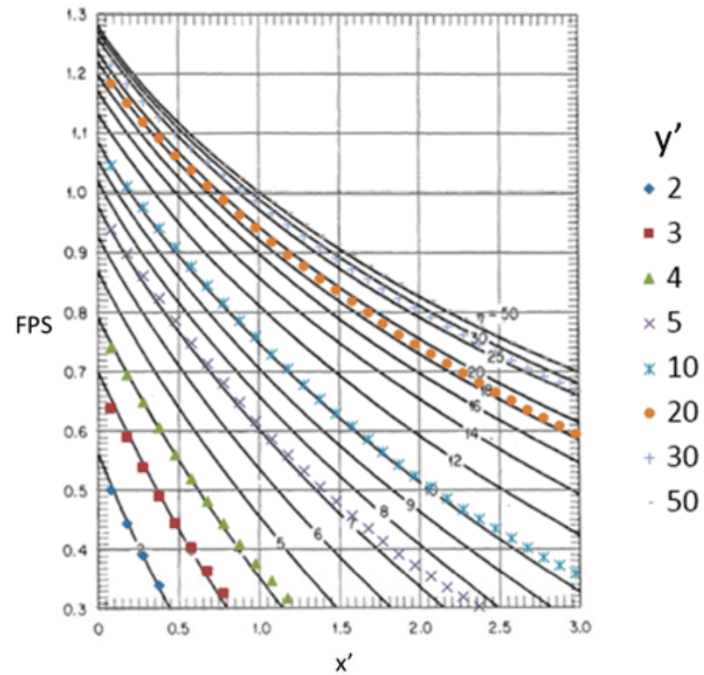

Figure 4 Parameterization of the F_{PS} adimentional function for planar channeling

$$F_{PS} = F_{PSo}\exp(-x'^{p}/g) \qquad (3.32)$$

$$F_{PSo} = 1.27(1 - exp(-y'^{0.76}/3.0) \qquad (3.33)$$

$$g = 4.3(1 - exp(-y'^{1.1}/12) \qquad (3.34)$$

$$p = 0.4exp(-y'/12) + 0.85 \qquad (3.35)$$

$\psi^{p}_{1/2}$ can then be calculated from Equation 3.21: $\psi^{p}_{1/2} = 0.72 F_{PS}(x', y')\psi_a$

3.2.2 Planar χ_{min} minimum yield/dechanneling probability

$$\chi_h^{[hkl]} = \frac{2a}{d_p^{[hkl]}} . \qquad (3.36)$$

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Comparison with experimental ½ angle results in handbooks

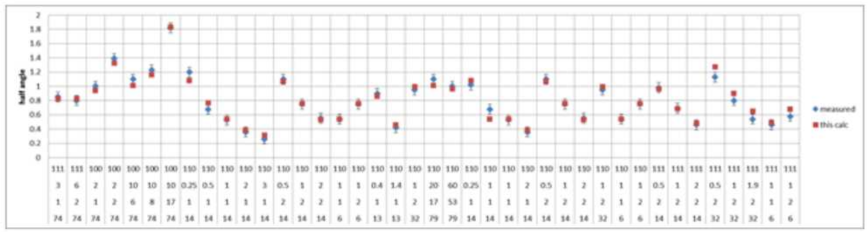

Figure 5 Measured half-angles in the IBA Handbooks of axial channeling compared to the calculations using the parameterizations developed here

In Figure 5, the numbers along the abscissa correspond from top to bottom to the <uvw> of the axis, the energy (MeV) and atomic number of the ion, and the atomic number of the target atoms. The best fit to this data was obtained with the equation:

$$\psi_{1/2}^{a} = 0.87 F_{RS}(x')\psi_1 \tag{4.1}$$

For planar channeling the same analysis was done with all the data presented in Reference [5], and the prefactor of planar channeling adjusted to obtain the best fit. This resulted in the following figure and analysis:

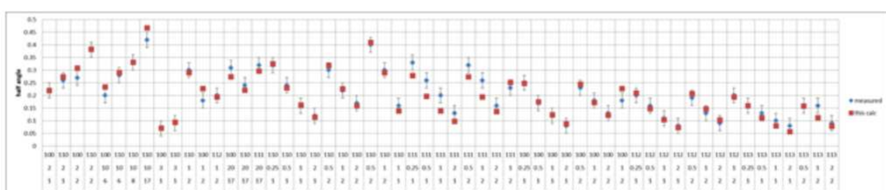

Figure 6 Measured half-angles in the IBA Handbooks for planar channeling compared to the calculations using the parameterizations developed here.

In Figure 6, the numbers along the abscissa correspond from top to bottom to the [hkl] of the plane, the energy (MeV) and atomic number of the ion, and the atomic number of the target atoms. The best fit to this data was obtained with the equation:

$$\psi_{1/2}^{p} = 0.65 F_{PS}(x', y')\psi_a \tag{4.2}$$

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http://www.sandia.gov/pcnsc/departments/iba/ibatable.html

Single click on a table element for IBA detail.

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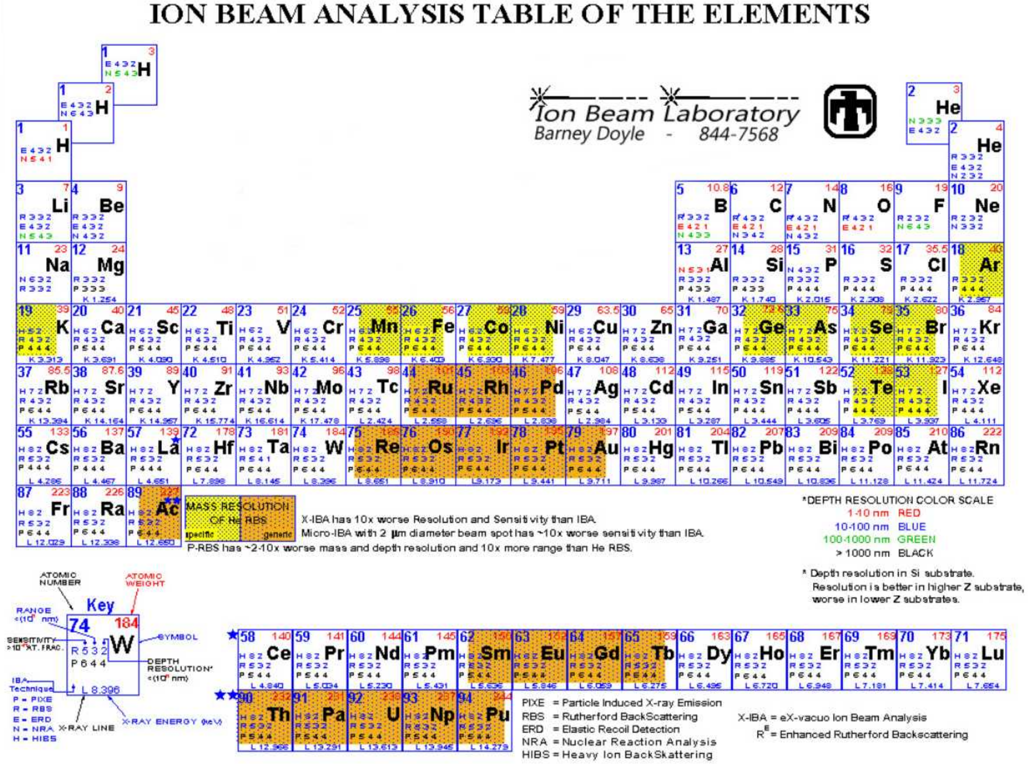

Top of table

Top of page

Related IBA Links:

Nuclear Physics Data:
TUNL Nuclear Data Evaluation

- SIGMACALC
- IBANDL

Data Analysis:

- RUMP
- SIMNRA

Ion Solid Interactions:

- SRIM
- DEDX (50K Excel file)
- Q (49K Excel file)
- IBA (81K Excel file)

Point of Contact: Barney L. Doyle

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