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Parameterization of Ion Channeling Half-Angles and Minimum Yields*

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Abstract

A MS Excel program has been written that calculates ion channeling half-angles and minimum yields in cubic bcc, fcc and diamond lattice crystals. All of the tables and graphs in the three Ion Beam Analysis Handbooks that previously had to be manually looked up and read from were programed into Excel in handy lookup tables, or parameterized, for the case of the graphs, using rather simple exponential functions with different power functions of the arguments. The program then offers an extremely convenient way to calculate axial and planar half-angles, minimum yields, effects on half-angles and minimum yields of amorphous overlayers. The program can calculate these half-angles and minimum yields for <uvw> axes and [hkl] planes up to (555).

1. INTRODUCTION

The three Ion Beam Analysis (IBA) Handbooks [1,2,3] have been an extremely useful references to practitioners of these techniques. However, because they first came out when powerful desk top computers were not available, many of the calculations still must involve the 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 strives to ameliorate this situation, at least for ion channeling, by presenting the background for a program that has been developed at Sandia National Laboratories that has been programed in universally available MS Excel, together with macros in Visual Basic Applications (VBA), making it facile to calculate channeling half angles $\psi_{1/2}$ and minimum yields $\chi_{\min}$. This report is intended to document the parameterizations and lookup tables that have been made, and accompany the program as a guide.

There has been a resurgence of interest in ion channeling. From the standpoint of ion beam analysis (IBA) one example includes the use of backscattering of finely focused and scanned low energy He ions from a He-Ion Microscope (HIM) [7] to observe the crystalline texture of poly/nano crystalline materials, much like is done with the analysis of Kikuchi patterns used by the electron backscatter diffraction (EBSD) technique. Ion channeling is also becoming of interest to materials scientists as regards the effect of unintentional channeling of ions used to simulate neutron induced displacement damage in polycrystalline materials [8], and intentional channeling to improve the sidewall roughness of ion-sputtered craters [9]. If the ions accidentally channel in individual crystallites in polycrystalline materials, 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.

This paper is focused on the automated analytical calculation of channeling half angles $\psi_{1/2}$ and minimum yields $\chi_{\min}$. A follow-on paper is planned that will treat accidental or unintentional channeling in textured polycrystalline materials. The approach involves reproducing all the tables in the channeling chapters of the three IBA handbooks into convenient tables in MS Excel where the Lookup command can be used to retrieve the necessary beam and material target parameters. In addition to the tables, all four of the theoretical calculations presented graphically in these handbooks have been parameterized with simple exponential functions where the argument of the exponential is taken to various power functions, in order to fit the calculations presented in the graphs. New rules for determining interatomic distances between rows of atoms along axes, and separation of atomic planes, both of which are needed for all these calculations, are introduced. The Excel program can calculate these half-angles and minimum yields for <uvw> axes and [hkl] planes up to (555).

2. THE CHANNELING EQUATIONS AND THEIR PARAMETERIZATION

We will not be re-deriving the channeling theories developed by Lindhard nearly 50 years ago, nor the supplements to his theory over the years, as all of this information is readily available in any of the IBA Handbooks. We will, however reproduce the equations that appear in Swanson's Appendix 15 [5] in the second Handbook [2], as this provides the most convenient collection of all the equations used in channeling half-angles $\psi_{1/2}$ and dechanneling probabilities $\chi_{\min}$.

2.1 Axial Channeling

2.1.1 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]:

$$\psi_1 = \sqrt{\frac{2Z_1Z_2e^2}{Ed}}\ (radians)\ , \tag{2.1}$$

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^2 is the square of the fundamental electron charge which equals $1.44\text{x}10^{-5}$ MeV-*Å* and *d* is the interatomic separation of the atoms in *Å* along the axial direction <uvw>.

$$d = f_a cc \tag{2.2}$$

The values for the factors, f_a, by which the conventional cell lattice constant (cc) needs to be multiplied to calculate *d,* are given in Table A15.1 in [5] for bcc, fcc and diamond lattices, but only up to <111> axes. The determination of these factors is actually fairly complicated. After entering Z_2 in the program, a lookup table is used to find the conventional cell lattice constant, cc, in *Å* and the symmetry of the crystal lattice, i.e. bcc, hcp or diamond. For now only cubic lattices are considered. When a <uvw> axial direction is entered, the program calculates the vectors to all the atoms with vector lengths less than that of <uvw> and checks for alignment with <uvw>. It then calculates d using the axial lattice constant factor:

$$f_a = \frac{\sqrt{u^2 + v^2 + w^2}}{1 + N}\ , \tag{2.3}$$

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. As a simple example, for bcc, *N*=1 for the <111> axis. *d* for each <uvw> axes is calculated by multiplying the corresponding f_a factor by the conventional cell lattice constant.

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

$$u_1 = 12.1 \left(\left(\frac{\phi_D(x'')}{x''} + 0.25 \right) \left(\frac{1}{M_2 \theta_D} \right) \right)^{1/2} \quad (\text{Å}), \tag{2.4}$$

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

$$x'' = \frac{\theta_D}{T} \ . \tag{2.5}$$

$\phi_D(x'')$ is the Debye function, which has been parameterized here to be:

$$\phi_D(x'') = \exp(-x''/4.3) \tag{2.6}$$

The fit to the Debye function plotted in A15.1 in [5] using this equation is shown in Fig. 1.

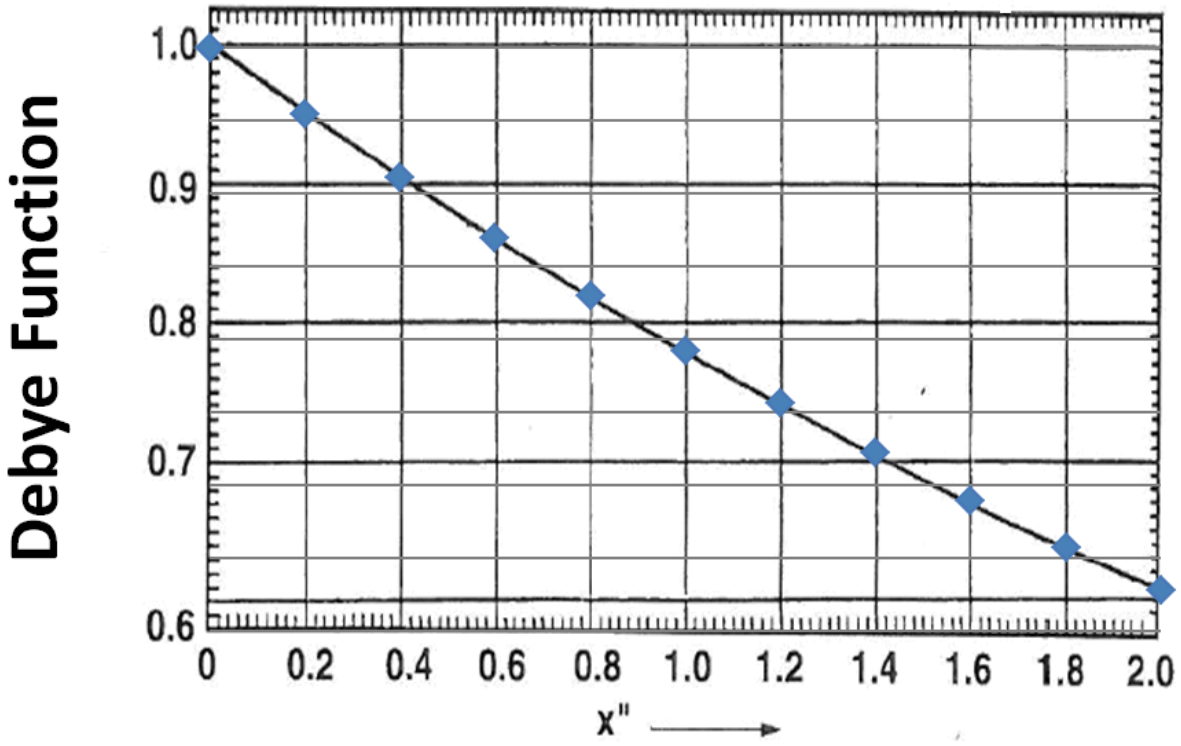

Figure 1. Parameterization (diamonds) of Debye Function (solid line).
Taken from figure A15.1 in reference [5].

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

$$x' = 1.2\frac{u_1}{a} \tag{2.7}$$

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]:

$$a = 0.04685 / (Z_1^{2/3} + Z_2^{2/3})^{1/2}\ \text{Å} \tag{2.8}$$

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

$$\psi_{1/2} = 0.8F_{RS}(x')\psi_1 \text{ for } \psi_1(rad) < \frac{a}{d} \tag{2.9}$$

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.

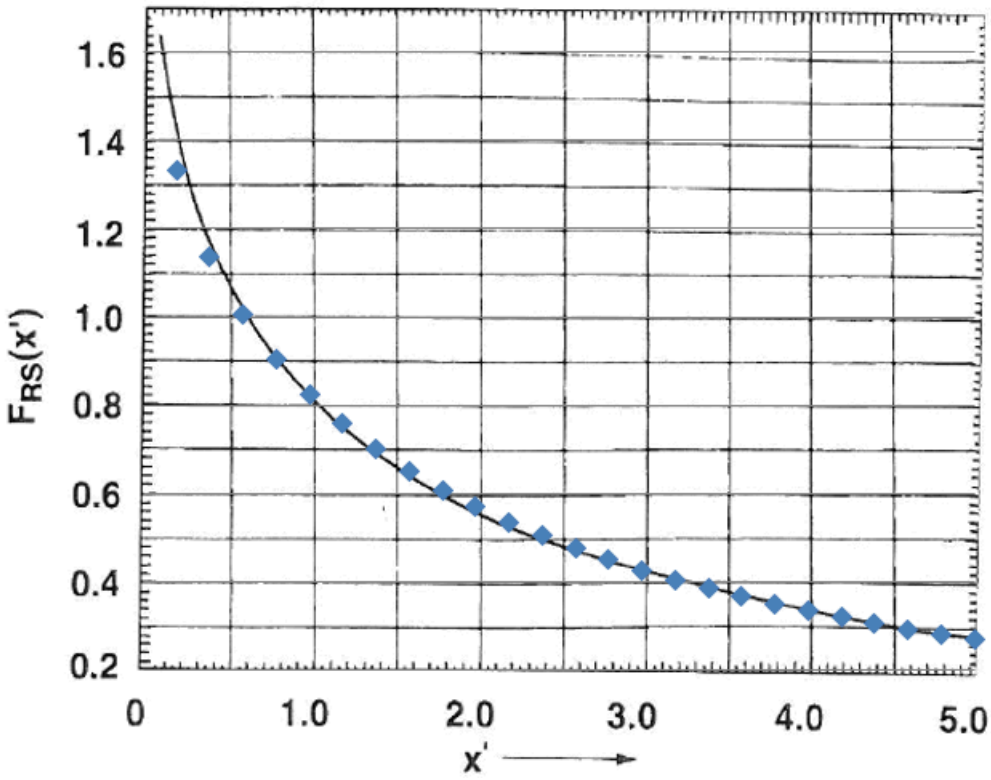

Figure 2. Parameterization (diamonds) of Barrett's F_{RS} adimensional function (solid line) for axial channeling. Taken from Figure A15.2 in reference [5].

The functional form of this parameterization was found to be given by:

$$F_{RS} = 1.9\exp(-x'^{0.53}/1.2) \tag{2.10}$$

Another expression for the axial half-angle is:

$$\psi_{1/2} = 7.57\sqrt{\frac{a\psi_1}{d}} \quad \text{for} \quad \psi_1(rad) > \frac{a}{d}\ , \tag{2.11}$$

2.1.2 Axial $\chi_{\min}$ minimum yield

Two equations are given in [5] for the axial $\chi_{\min}$. The first was derived by Lindhard [10] :

$$\chi_h^{<uvw>} = Nd\pi\left(2u_1^2 + a^2\right) , \tag{2.12}$$

and the second by Barrett [12] which is:

$$\chi_h^{<uvw>} = 18.8Ndu_1^2\sqrt{1+\frac{1}{\xi^2}} , \tag{2.13}$$

where

$$\xi = 126\frac{u_1}{\left(\psi_{1/2}d\right)} \tag{2.14}$$

Barrett's equations are used for the axial $\chi_{\min}$ in this paper and the program.

2.*1.3 Effect of amorphous overlayers on axial channeling*

Not all crystals used as targets for channeling experiments are perfect all the way to the surface. Many have amorphous overlayers, e.g. the 15 $\mathring{A}$ SiO_2 native oxide on the surface of Si. In addition, there is the use of Si implants into Si microelectronics to amorphize the near surface in order to avoid unwanted channeling that increases the junction depths of very shallow dopant implants. The effect of these overlayers was addressed and theoretically analyzed by Lugujjo and Mayer in their landmark paper in 1973 [13]. The equations and graph they derived for calculating the effect of these overlayers are included in Swanson's Appendix [5], and the graphical information is parameterized here.

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

$$\theta_c = \frac{a_{13}E\psi_{1/2}}{\left(2Z_1Z_3e^2\right)} , \tag{2.15}$$

where Z_3 is the atomic number of the overlayer. We point out here that the equations in all three IBA handbooks [1,2,3] are wrong, because they do not agree with the Lugujjo and Mayer paper. This is because in all three Handbooks the Z_3 term in Equation 3.14 above, has been replaced by Z_2 and the value of *a* in equation 3.14 should be calculated for the Thomas-Fermi screening distance given for the incident ion in the overlayer, i.e.:

$$a_{13} = 0.04685 / (Z_1^{2/3} + Z_3^{2/3})^{1/2} \tag{2.16}$$

Now this is probably justified in the case of the native oxides or certainly Si amorphized layers on Si crystals, but the Lugujjo and Mayer paper derived expressions for the overlayer's effect on the channeling angle that was more generally applicable, i.e. for any overlayer of atomic number Z_3.

The increase in minimum yield $\chi_h^{<uvw>}$ is given by:

$$\chi_{\min} = P(\theta_c), \tag{2.17}$$

where the P function was given in graphical form in [13]. As in the previous cases where this information was graphical, we have parameterized $P(\theta_c)$, and in Figure 4 we show the results of that parameterization.

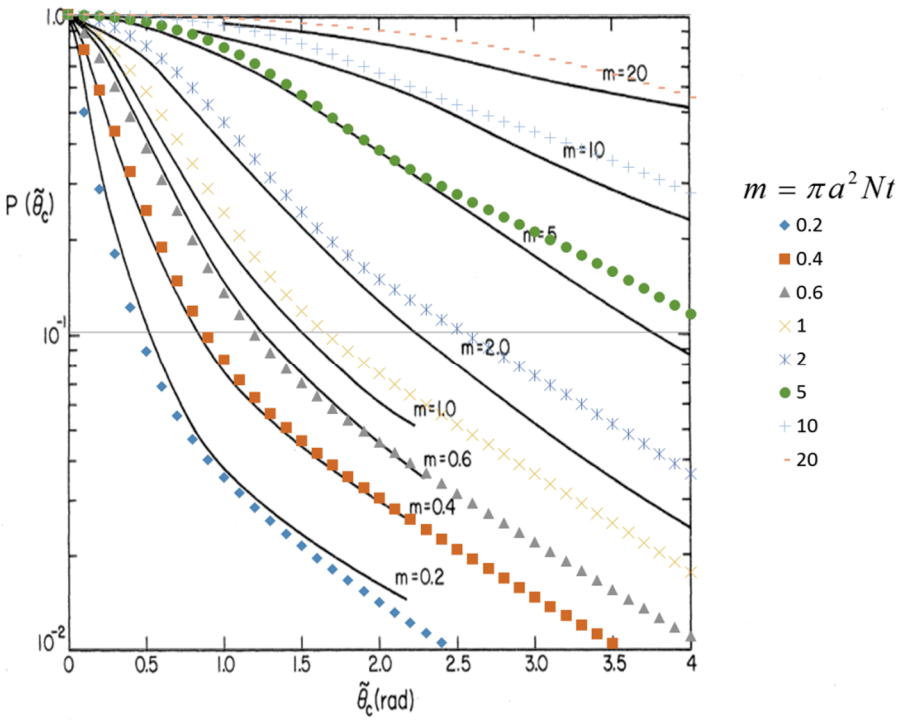

Figure 3. P function (solid lines) describing dechanneling due to amorphous overlayers together with the parameterization presented here (various symbols in the legend). Taken from Lugujjo and Mayer [13] .

In this parameterization the overlayer thickness parameter m is given by:

$$m = \pi a^2 Nt \tag{2.18}$$

Where a is the Thomas-Fermi screening distance given in Equation 2.16, N is the concentration of overlayer atoms per $\mathring{A}^3$ and t is the thickness in $\mathring{A}$. To check the accuracy of our parameterization of P, we compare to an example given in the Appendix of Ref. [13] for 1.8 MeV He^+ on <110> Si with two different overlayers.

	Overlayer	
1.8 MeV He->110 Si	**1550A Al**	**440A Au**
P(thc,m)= (this work)	0.22	0.61
P=(Ref. [13])	0.20	0.57

Table 1 Comparison of P(θ_c) from this parameterization and the example given in the Appendix of Ref. [13]

2.2 Planar Channeling

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

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

$$\psi_{1/2}^{p} = 0.72 F_{PS}\left(x', y'\right)\psi_a \ , \tag{2.19}$$

where

$$\psi_a = 0.545\sqrt{\frac{Z_1 Z_2 N d_p a}{E}} \ \ (degrees) \ . \tag{2.20}$$

N is the concentration of target atoms in units of $\#/\mathring{A}^3$ and d_p is the interatomic separation of the planes ($\mathring{A}$) for the usual [hkl] Miller index orientations, and Table A15.1 in [5] gives multiplicative factors for the lattice constants (cc) to get these separations, again for bcc, fcc and diamond lattices, but only up to [111].

$$d_p = f_p cc \tag{2.21}$$

The calculation of the interatomic separation of crystalline planes d_P from the standpoint of ion channeling is quite different from that for x-ray diffraction. This is because the coordinate system for diffraction is in reciprocal space, while that for channeling is in real space.

For bcc lattices, this factor is:

$$f_p^{bcc} = \frac{1}{\sqrt{h^2 + k^2 + l^2}} \ \text{for} \ h + k + l = even \ , \tag{2.22}$$

or

$$f_p^{bcc} = \frac{1}{2\sqrt{h^2+k^2+l^2}} \text{ for } h+k+l = odd \ . \tag{2.23}$$

For fcc lattices, this factor becomes:

$$f_p^{fcc} = \frac{1}{\sqrt{h^2+k^2+l^2}} \text{ for } h,k,l \text{ all odd} \ , \tag{2.24}$$

or

$$f_p^{fcc} = \frac{1}{2\sqrt{h^2+k^2+l^2}} \text{ for } h,k,l = \text{ not all odd} \ . \tag{2.25}$$

For diamond lattices, the factor is:

$$f_p^{fcc} = \frac{1}{2\sqrt{h^2+k^2+l^2}} \text{ for all } h,k,l \text{ except permutations of } [001] \tag{2.26}$$

or

$$f_p^{fcc} = \frac{1}{4} \text{ for all permutations of } [001] \text{ e.g. } [010], [00\bar{1}] \text{ etc.} \tag{2.27}$$

d_p is then determined by multiplying the associate [hkl] factor by the conventional cell lattice constant (cc) as in equation 2.21.

$F_{PS}(x',y')$ in equation 2.19 is the square root of the adimensional planar potential using Moliere's screening function and also calculated using Monte Carlo techniques by Barrett [12]. The arguments in F_{PS} are:

$$x' = 1.6\left(\frac{u_1}{a}\right) \text{, and} \tag{2.28}$$

$$y' = \frac{d_p}{a} \tag{2.29}$$

The parameterized fit to the F_{PS} function plotted in A15.3 in [5] is shown in Fig. 4.

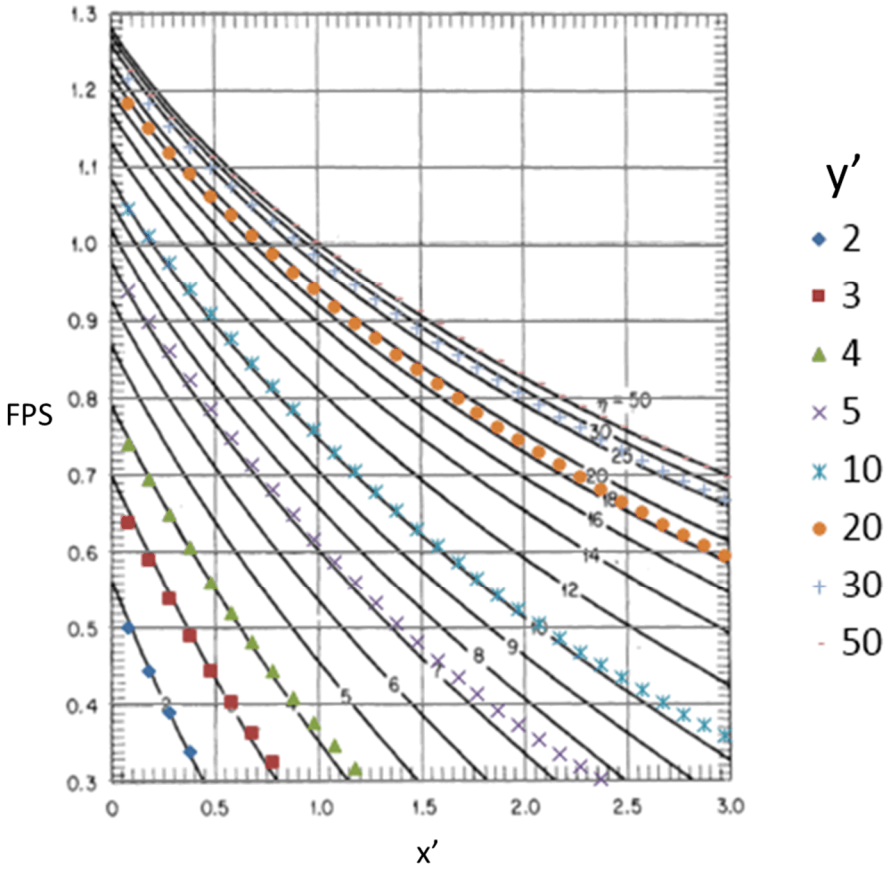

Figure 4. Parameterization (various symbols in legend) of Barret's F_{PS} adimentional function (solid lines) for planar channeling. Taken from Figure A15.3 in reference [5].

The equations used in this parameterization of the F_{PS} function are:

$$F_{PS} = F_{PSo} \exp(-x'^{p} / a) \tag{2.30}$$

$$F_{PSo} = 1.27(1 - exp(-y'^{0.76} / 3.0) \tag{2.31}$$

$$a = 4.3(1 - exp(-y'^{1.1} / 12) \tag{2.32}$$

$$p = 0.4exp\left(-y'/12\right) + 0.85 \tag{2.33}$$

$\psi_{1/2}^{p}$ can then be calculated from Equation 2.19 .

2.2.2 Planar $\chi_{\min}$ minimum yield/dechanneling probability

The equation given in [5] for the planar $\chi_{\min}$ was derived by Lindhard [10] and is:

$$\chi_h^{[hkl]} = \frac{2a}{d_p^{[hkl]}} \quad . \tag{2.34}$$

3. COMPARISON WITH EXPERIMENTAL HALF-ANGLES GIVEN IN THE HANDBOOKS

The IBA Handbooks have a considerable amount of half-angle and minimum yield data generated by many of the researchers in the field. These measurements have been compared to the parametric calculations described above. The calculation of parameterized half-angles is compared to the axial channeling data presented in [5] in Table A15.5 and in Figure 5 below.

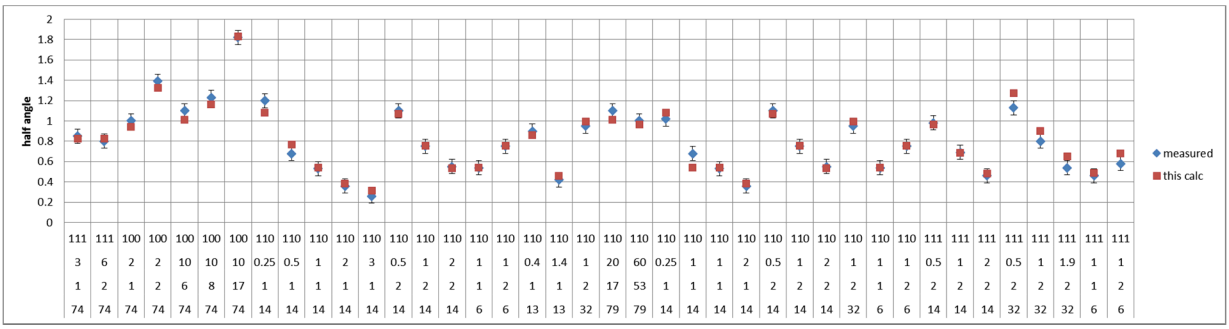

Figure 5 Measured half-angles in the IBA Handbooks (diamonds) of axial channeling compared to the calculations using the parameterizations developed here (squares). Taken from Table A15.5 in reference [5].

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. It should be pointed out that in order to get the best fit to the data plotted above, the prefactor was adjusted to be 0.87 so that the reduced χ_α^2 was 0.74 and the recommended equation for the axial channeling half-angle given here is therefore:

$$\psi_{1/2}^a = 0.87 F_{RS}(x')\psi_1 \tag{3.1}$$

For planar channeling the same analysis was done with all the data presented in Table A15.6, reference [5], and the prefactor of planar channeling adjusted to obtain the best fit. This resulted in plots in Figure 6 :

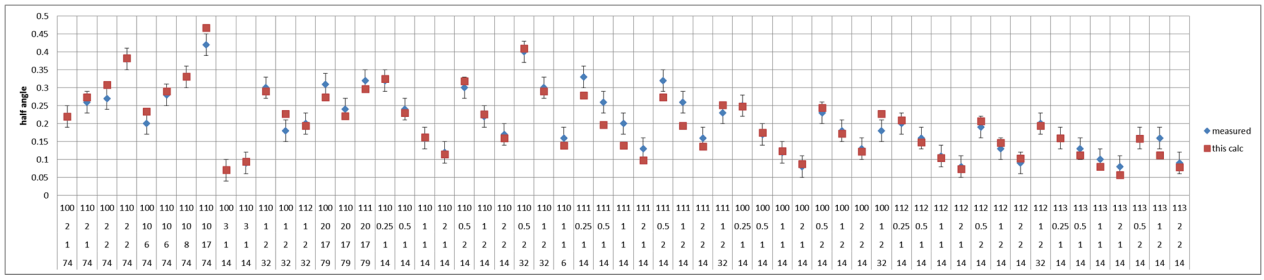

Figure 6 Measured half-angles in the IBA Handbooks for planar channeling (diamonds) compared to the calculations using the parameterizations developed here (squares). Taken from Table A15.6 reference [5].

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. As with the axial channeling calculations and their comparisons with the data presented in [5], the prefactor was adjusted to get the best fit, and this resulted in the best equation to use for calculating the planar channeling half-angle to be:

$$\psi_{1/2}^{p} = 0.65 F_{PS}\left(x', y'\right)\psi_a \tag{3.2}$$

The prefactors used in Equations 3.1 and 3.2 are therefore those used in the program.

4. CONCLUSIONS

This paper gives all the equations and parameterization of graphical representations of Monte-Carlo calculations of ion channeling to determine the half-angles for axial and planar channeling and their minimum yields. A program has been developed in universally available MS Excel together with macros in Visual Basic Applications (VBA) to perform these calculations. The program uses all the equations both derived from basic physics by Lindhard [10] and those parameterized here from Barrett's Monte-Carlo calculations [12] . The program can calculate the axial and planar half-angles for channeling given only the atomic number and energy of the projectile, and the atomic number of the target. The indices of these axes and planes can go up to (555), as this seem a practical limit to the use of the channeling equations and parameterized graphs.

The impetus for these calculations was a paper written in collaboration with Sandia by El-Atwani et. al [8] where the effects of ion channeling on the reduction of MeV-energy heavy ions on nanocrystalline samples of W studied with Sandia's unique in-situ ion irradiation TEM (I^3TEM). The I^3TEM was used to observe the accumulation of such damage in real time. This report concluded that ion channeling may dramatically reduce the effects of displacement damage by the recoil of polycrystalline material atoms. A Sandia Report [14] has been prepared that discusses the use of the parameterized channeling equations and program presented here for calculating

stereographic projections of ion channeling and accidental, or unintentional, channeling probabilities and how this can affect the interpretation of ion-simulated neutron damage.

The MS Excel program is open source and available at http://www.sandia.gov/pcnsc/departments/iba/ibatable.html . The program is simply named channeling.xlsm .

5. ACKNOWLEDGEMENTS

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