Calculations of Unintentional Axial and Planar Ion Channeling in Polycrystalline Solids

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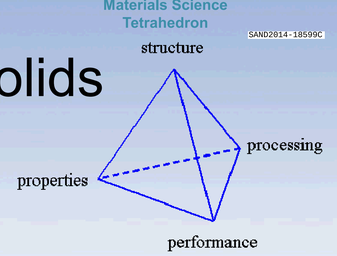
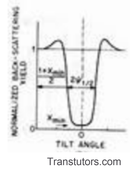


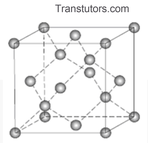
Channeling

- Ion channeling has been used for over 50 years to better the atomic-level understanding of the structure of single crystals.
- Channeling typically involves measuring the backscatter intensity of a parallel beam of MeV-energy ions directed onto a crystal whose orientation is changed with a precision goniometer.
- Details of crystal structure, such as the 3D position of interstitial atoms, can then be resolved with sub-*Å* resolution.
- …but unintentional ion channeling can lead to unexpected results when using high energy ions to simulate the production of neutron damage in polycrystalline materials, such as those used in current fission and future fusion nuclear reactors.
- Some nano-grains can experience less displacement damage than neighboring grains depending on their orientation to the ion beam, and this is thought to affect mechanical properties.

Purpose of This Report

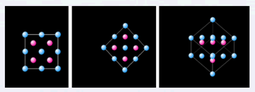
- To write an Excel program that calculates the "half-angles" and "minimum yields" for all the important axial and planar channeling orientations of any ion at any energy for any material with body-centered cubic, face-centered cubic, and diamond lattice crystal structures.
- … and use these results to calculate unintentional axial and planar channeling probabilities of MeV energy ions being used in the Ion Beam Laboratory at Sandia to simulate the effects of high energy neutrons on material systems.
- Previously, these calculations were laborious, and now they are easily made.

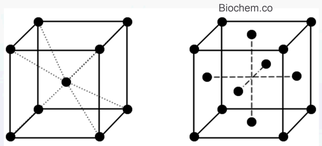




Diamond Lattice Crystal Structure

Diamond Lattice Channeling





Body-Centered Cubic and Face-Centered Cubic Crystal Structures

The Equations

- The equations used to calculate channeling half-angles were obtained from Chapter 10 and Appendix 15 (M. L. Swanson), of the *Handbook of Modern Ion Beam Materials Analysis* (edited by J. Tesmer, M. Nastasi, J. Barbour, C. Maggiore, and J. Mayer).
- To evaluate the equations it was necessary to parameterize several curves in Appendix 15 that were originally generated using Monte-Carlo simulations of channeling by John Barrett in 1971. Previously one had to manually read the values of these curves from graphs!

The Calculations

Axial Channeling

Jens Lindhard derived the theory for axial and planar channeling angles 50 years ago. The characteristic axial channeling angle is given in the equation:

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

Where Z_1 is the atomic number of the projectile, E is the energy (MeV) of the projectile, Z_2 is the atomic number of the target atoms, e^2 is the fundamental electron charge squared which equals 1.44x10^{-5} MeV-*Å* and *d* is the separation of the atoms in *A* along the axial direction <uvw> given in the usual Miller indices.

The expressions for axial channeling half-angles are given as:

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

and

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

Where the function F_{RS} was parameterized, and a is the Thomas-Fermi screening length, and is given as

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

Planar Channeling

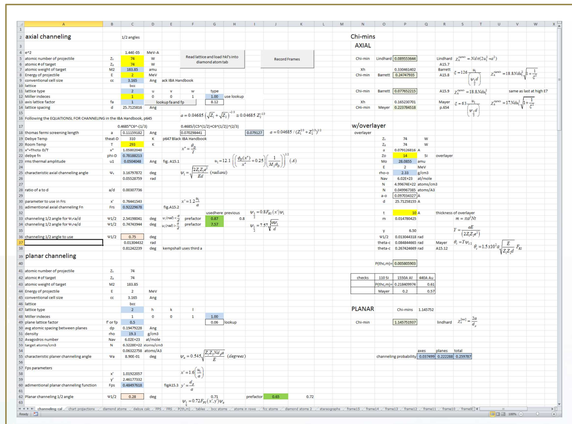
The planar half-angles are given in the equation:

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

where

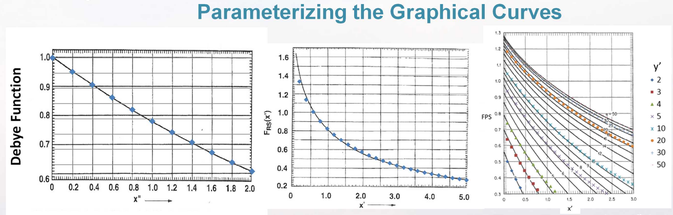
$$\psi_a = 0.545\sqrt{\frac{Z_1Z_2Nd_pa}{E}}\ (degrees)$$

and N is the concentration of target atoms and d_p is the atomic separa of the planes (Å). The function F_{PS} was parameterized to solve for the angles.



The equations along with the variables were put into a Microsoft Excel spreadsheet and the process of automating the calculations was done through Excel. Each variable was accounted for, inputted, then plugged into the original channeling equations to find the probability of unintentional channeling.

Parameterizing the Graphical Curves



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

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

$$F_{PS} = F_{PS0}\exp(-x'^{p}/a)$$
$$F_{PS0} = 1.27(1-exp(-y'^{0.76}/3.0))$$
$$a = 4.3(1-exp(-y'^{1.1}/12))$$
$$p = 0.4exp(-y'/12) + 0.85$$

To parameterize the Debye function, the F_{RS} function, and the F_{PS} function, the graphs that previously had to be read manually were scanned and used to find functions that matched the ones on the graph. The functions were found by matching up plot lines to the original graphs.

The Program

It was necessary to input a table in which each target element was associated with its atomic number, structure, Debye temperature, and lattice constant. This was implemented to automatically enable the user to look up the values needed for the calculations.

element	Z	mass	density	structure	Debye
H	1	1.008	0.0899		
He	2	4.003	0.1787		
Li	3	6.941	0.53		
Be	4	9.012	1.85		
B	5	10.810	2.34		
C	6	12.011	2.62	diamond	20
N	7	14.007	1.251		
O	8	15.999	1.429		
F	9	18.998	1.696		
Ne	10	20.179	0.901		
Na	11	22.990	0.97		
Mg	12	24.305	1.74		
Al	13	26.982	2.7	fcc	3
Si	14	28.086	2.33	diamond	5
P	15	30.974	1.82		
S	16	32.060	2.07		
Cl	17	35.453	3.17		
Ar	18	39.948	1.784		
K	19	39.098	0.86		
Ca	20	40.080	1.55		
Sc	21	44.956	3		
Ti	22	47.900	4.5		
V	23	50.942	5.8	bcc	360
Cr	24	51.996	7.19	bcc	485
Mn	25	54.938	7.43		
Fe	26	55.847	7.86	bcc	420
Co	27	58.933	8.9		
Ni	28	58.700	8.9	fcc	425
Cu	29	63.546	8.96	fcc	315
Zn	30	65.390	7.14		
Ga	31	69.720	5.91		
Ge	32	72.590	5.32	diamond	290
As	33	74.922	5.72		
Se	34	78.960	4.8		
Br	35	79.904	3.12		
Kr	36	83.800	3.74		
Rb	37	85.468	1.53		
Sr	38	87.620	2.6		
Y	39	88.906	4.5		
Zr	40	91.220	6.49		
Nb	41	92.906	8.55	bcc	275
Mo	42	95.940	10.2	bcc	380
Tc	43	98.000	11.5		
Ru	44	101.070	12.2		
Rh	45	102.906	12.4	fcc	340
Pd	46	106.400	12	fcc	275
Ag	47	107.868	10.5	fcc	215
Cd	48	112.410	8.65		
In	49	114.820	7.31		
Sn	50	118.690	7.3		
Sb	51	121.750	6.68		
Te	52	127.600	6.24		
I	53	126.905	4.92		
Xe	54	131.300	5.89		
Cs	55	132.905	1.87		
Ba	56	137.330	3.5		
La	57	138.906	6.7		
Ce	58	140.120	6.78		
Pr	59	140.908	6.77		
Nd	60	144.240	7		
Pm	61	145.000	6.475		
Sm	62	150.400	7.54		
Eu	63	151.960	5.26		
Gd	64	157.250	7.89		
Tb	65	158.925	8.27		
Dy	66	162.500	8.54		
Ho	67	164.930	8.8		
Er	68	167.260	9.05		
Tm	69	168.934	9.33		
Yb	70	173.040	6.98		
Lu	71	174.967	9.84		
Hf	72	178.490	13.1		
Ta	73	180.948	16.6	bcc	245
W	74	183.850	19.3	bcc	310
Re	75	186.207	21		
Os	76	190.200	22.4		
Ir	77	192.220	22.5		
Pt	78	195.090	21.4	fcc	225
Au	79	196.967	19.3	fcc	170
Hg	80	200.590	13.53		
Tl	81	204.370	11.85		
Pb	82	207.200	11.4	fcc	88
Bi	83	208.980	9.8		
Po	84	209.000	9.4		
At	85	210.000			
Rn	86	222.000	9.91		
Fr	87	223.000			
Ra	88	226.025	5		
Ac	89	227.028	10.07		
Th	90	232.038	11.7		
Pa	91	231.036	15.4		
U	92	238.029	18.9		

Stereographic Projections

The axial and planar ion channeling can be represented by the program in the form of stereographic projections. The equations used to create these projections for axial channeling are:

$$x = \frac{u}{\sqrt{u^2+v^2}}$$

$$y = \frac{v}{\sqrt{u^2+v^2}}$$

$$z = \frac{w}{\sqrt{u^2+v^2+w^2}}$$

$$\varphi = \tan^{-1}(y/x)\ ,$$

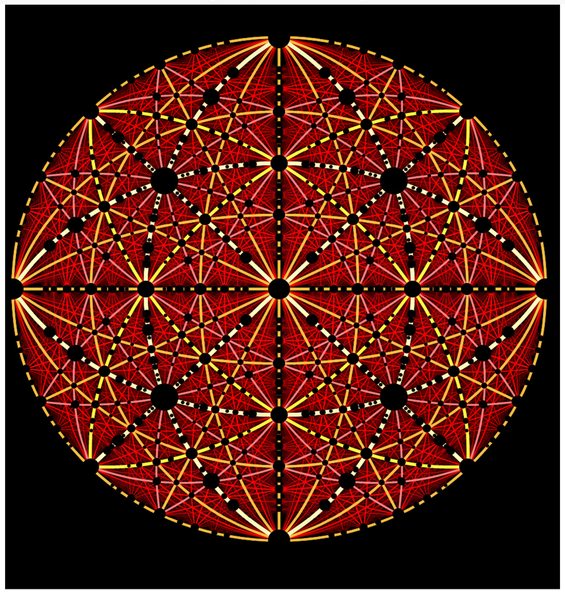
$$\theta = \cos^{-1}(z)$$

The position on the stereograph of an axial direction is then calculated using the following equations:

$$x' = x\theta$$

$$y' = y\theta\ ,$$

Stereographic Projection



2 MeV Si on <001> W

Research Applications

	channeling probability		
2 MeV	axes	planes	total
W->W	0.037	0.326	0.363
Cu->W	0.027	0.219	0.246
Si->W	0.020	0.157	0.178

Channeling probability for 2 MeV W, Cu and Si on W.

For the exposure conditions used by El-Atwani and Hattar to simulate neutron damage in W nanocrystals, there was a considerable amount of channeling occurring. How this relates to the accidental channeling that occurs with neutron exposures is unknown, and this needs to be a subject for further research.

Conclusions

A SAND Report has been written that 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 with these angles determine the accidental or unintended channeling of implanted ions, or those recoiled by neutrons an primary knock on atoms in polycrystalline metals in nuclear fission or future fusion reactors.

This report and the Excel program can be made available upon request. Contact bldoyle@sandia.gov.

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