



# Ion Channeling Revisited

SAND2015-5542C

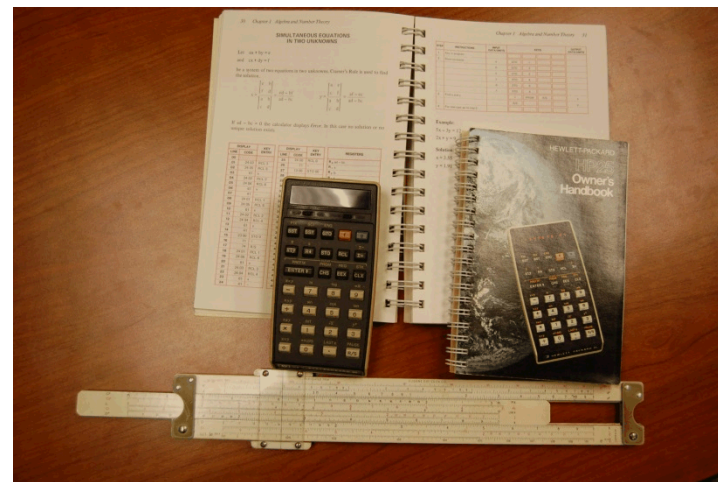
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# Why revisit channeling?

- 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.

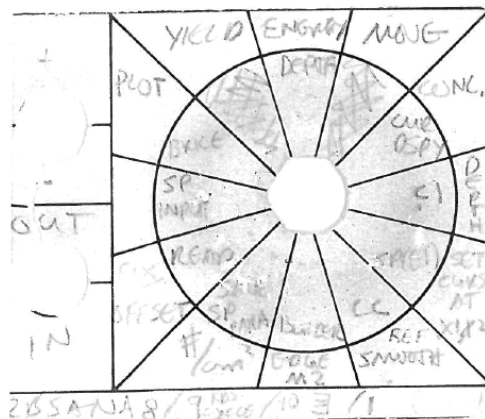
## This & That

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

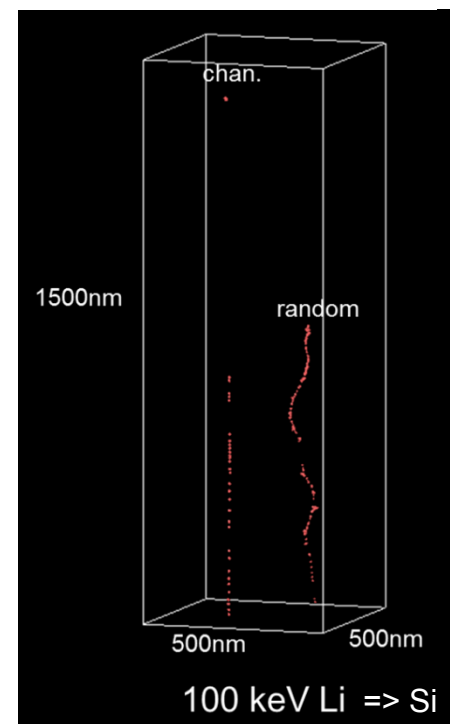
## LAB NEWS

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 $\psi_{12}$ half-angles

The specular or characteristic axial channeling angle  $\psi_1$  is calculated using the formula given in Lindhard's famous paper [10]:

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

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  $1.44 \times 10^{-5}$  MeV-Å and  $d$  is the separation of the atoms in  $A$  along the axial direction  $\langle uvw \rangle$ .

$$d = f_a cc \quad (3.2)$$

$cc$  is the conventional cell size and

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

where  $N$  is the number of atoms between and along the same direction as  $\langle uvw \rangle$ . 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:

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

Where  $\theta_D$  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

$$x'' = \frac{\theta_D}{T} . \quad (3.5)$$

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



# Debye Function

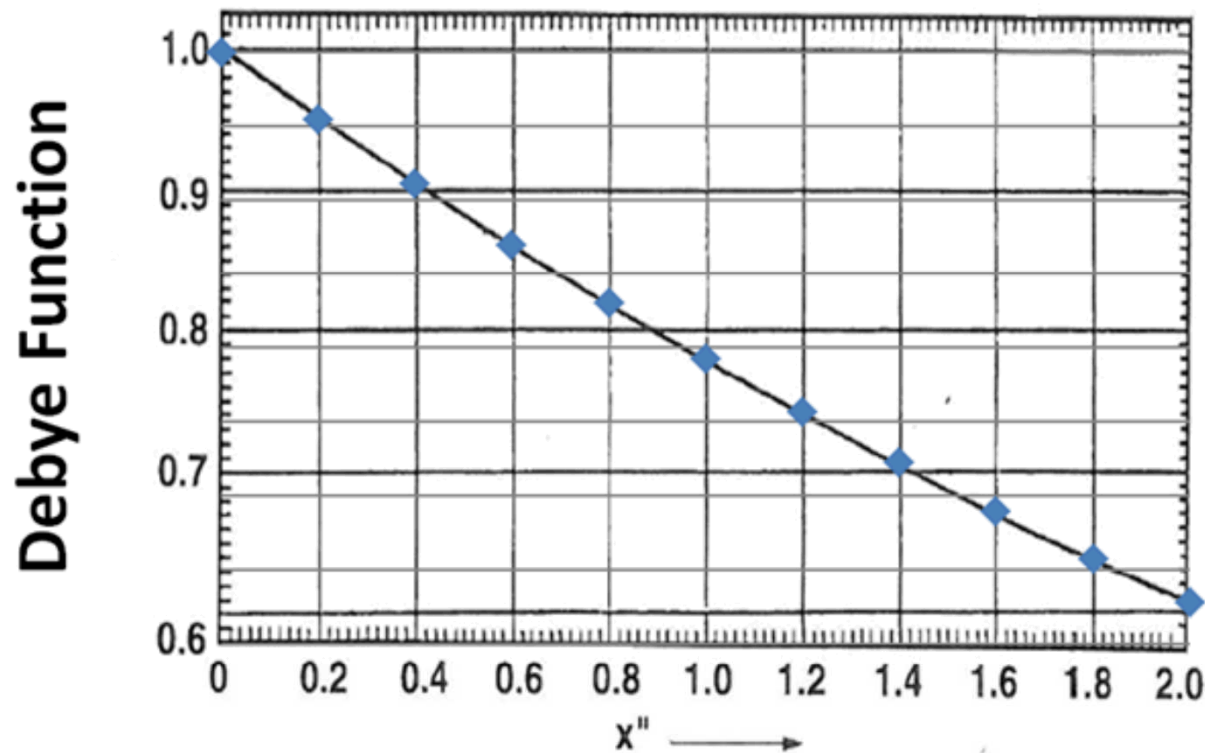


Figure 1 Parameterized Debye Function

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

(3.6)

# Channeling 1/2 angle and adimensional string function

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

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

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]:

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

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

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

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

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.

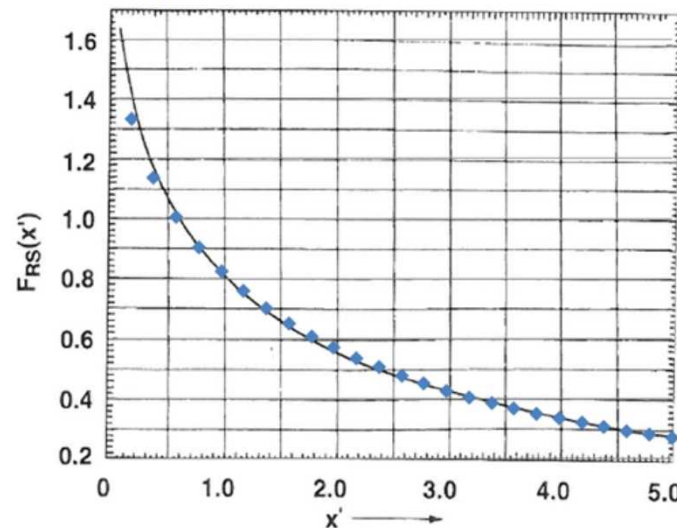


Figure 2 Parameterization of the  $F_{RS}$  adimensional function for axial channeling

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

# axial $\chi$ -min

## 3.1.2 Axial $\chi_{\min}$ minimum yield/dechanneling probability

In this report we are equating the  $\chi_{\min}$  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  $\chi_{\min}$ . The first is attributed to Lindhard [10]:

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

and the second to Barrett [12] which is:

$$\chi_h^{<unn>} = 18.8Ndu_1^2 \sqrt{1 + \frac{1}{\xi^2}} , \quad (3.13)$$

where

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

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



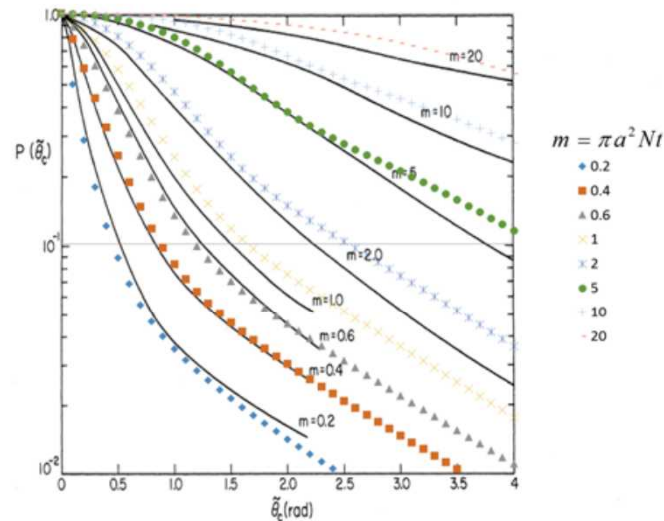
# Overlayers

## 3.1.3 Effect of amorphous overlayers on axial channeling

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

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

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



**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  $\text{\AA}^3$  and  $t$  is the thickness in  $\text{\AA}$

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

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

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

# 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:

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

where

$$\psi_a = \sqrt{\frac{2Z_1 Z_2 e^2}{E d_p}} \text{ (radians) } . \quad (3.22)$$

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

$$d_p = f_p cc \quad (3.23)$$

Where  $cc$  is the size of the conventional cell.

For bcc lattices, this factor is:

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

For fcc lattices, this factor becomes:

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

For diamond lattices, the factor is:

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

$F_{PS}(x', y')$  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].

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

$$y' = \frac{d_p}{a} \quad (3.31)$$

# planar 1/2 angle and adimensional planar function

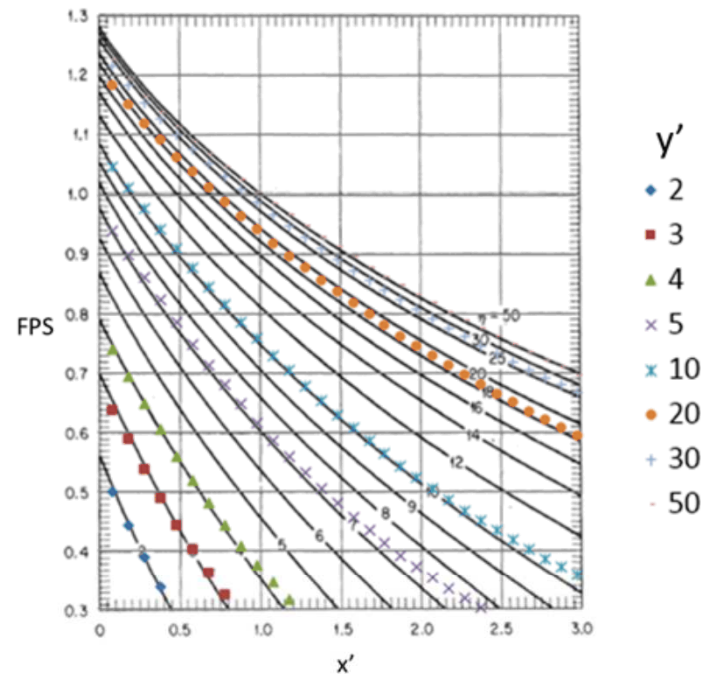


Figure 4 Parameterization of the  $F_{PS}$  adimensional function for planar channeling

$$F_{PS} = F_{PS0} \exp(-x'^p / g) \quad (3.32)$$

$$F_{PS0} = 1.27(1 - \exp(-y'^{0.76} / 3.0)) \quad (3.33)$$

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

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

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

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

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

(3.36)

# Comparison with experimental 1/2 angle results in handbooks

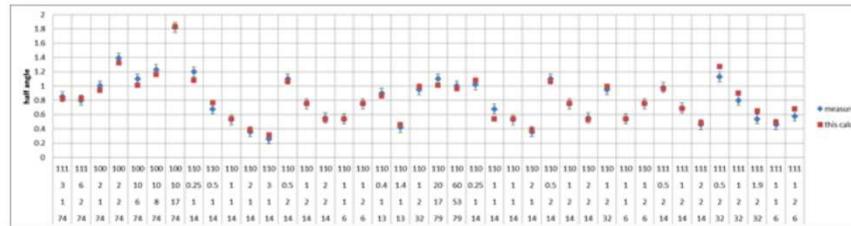


Figure 5 Measured half-angles in the IBA Handbooks of axial channeling compared to the calculations using the parameterizations developed here

In Figure 5, the numbers along the abscissa correspond from top to bottom to the  $\langle uvw \rangle$  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:

$$\psi_{12}^a = 0.87 F_{RS}(x') \psi_1 \quad (4.1)$$

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:

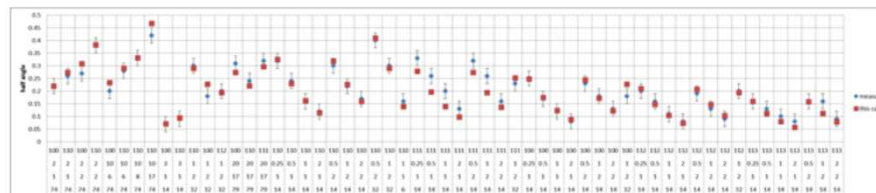


Figure 6 Measured half-angles in the IBA Handbooks for planar channeling compared to the calculations using the parameterizations developed here.

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:

$$\psi_{12}^p = 0.65 F_{PS}(x', y') \psi_a \quad (4.2)$$




Single click on a table element for IBA detail.

[Bottom of table](#)

## ION BEAM ANALYSIS TABLE OF THE ELEMENTS

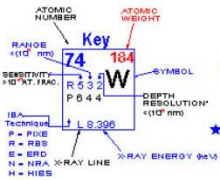
\*Ion Beam Laboratory  
Barney Doyle - 844-7568



1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20
H	He																		
3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
Li	Be	B	C	N	O	F	Ne												
11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30
Na	Mg	Al	Si	P	S	Cl	Ar												
39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58
K	Ca	Sc	Ti	V	Cr	Mn	Fe	Co	Ni	Cu	Zn	Ga	Ge	As	Se	Br	Kr		
57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76
Sr	Y	Zr	Nb	Mo	Tc	Ru	Rh	Pd	Ag	Cd	In	Sn	Sb	Te	I	Xe			
73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92
Cs	Ba	La	Ce	Pr	Nd	Pm	Sm	Eu	Gd	Tb	Dy	Ho	Er	Tm	Yb	Lu			
87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106
Fr	Ra	Ac	Th	Pa	U	Np	Pu	Am	Cm	Bk	Cf	Es	Fm	Md	Nb	Lr			

\*DEPTH RESOLUTION COLOR SCALE  
1-10 nm RED  
10-100 nm BLUE  
100-1000 nm GREEN  
> 1000 nm BLACK

\*Depth resolution in Si substrate.  
Resolution is better in higher Z substrate,  
worse in lower Z substrates.



58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99	100	101	102	103	104	105	106	107	108	109	110	111	112	113	114	115	116	117	118	119	120	121	122	123	124	125	126	127	128	129	130	131	132	133	134	135	136	137	138	139	140	141	142	143	144	145	146	147	148	149	150	151	152	153	154	155	156	157	158	159	160	161	162	163	164	165	166	167	168	169	170	171	172	173	174	175	176	177	178	179	180	181	182	183	184	185	186	187	188	189	190	191	192	193	194	195	196	197	198	199	200	201	202	203	204	205	206	207	208	209	210	211	212	213	214	215	216	217	218	219	220	221	222	223	224	225	226	227	228	229	230	231	232	233	234	235	236	237	238	239	240	241	242	243	244	245	246	247	248	249	250	251	252	253	254	255	256	257	258	259	260	261	262	263	264	265	266	267	268	269	270	271	272	273	274	275	276	277	278	279	280	281	282	283	284	285	286	287	288	289	290	291	292	293	294	295	296	297	298	299	300	301	302	303	304	305	306	307	308	309	310	311	312	313	314	315	316	317	318	319	320	321	322	323	324	325	326	327	328	329	330	331	332	333	334	335	336	337	338	339	340	341	342	343	344	345	346	347	348	349	350	351	352	353	354	355	356	357	358	359	360	361	362	363	364	365	366	367	368	369	370	371	372	373	374	375	376	377	378	379	380	381	382	383	384	385	386	387	388	389	390	391	392	393	394	395	396	397	398	399	400	401	402	403	404	405	406	407	408	409	410	411	412	413	414	415	416	417	418	419	420	421	422	423	424	425	426	427	428	429	430	431	432	433	434	435	436	437	438	439	440	441	442	443	444	445	446	447	448	449	450	451	452	453	454	455	456	457	458	459	460	461	462	463	464	465	466	467	468	469	470	471	472	473	474	475	476	477	478	479	480	481	482	483	484	485	486	487	488	489	490	491	492	493	494	495	496	497	498	499	500	501	502	503	504	505	506	507	508	509	510	511	512	513	514	515	516	517	518	519	520	521	522	523	524	525	526	527	528	529	530	531	532	533	534	535	536	537	538	539	540	541	542	543	544	545	546	547	548	549	550	551	552	553	554	555	556	557	558	559	560	561	562	563	564	565	566	567	568	569	570	571	572	573	574	575	576	577	578	579	580	581	582	583	584	585	586	587	588	589	590	591	592	593	594	595	596	597	598	599	600	601	602	603	604	605	606	607	608	609	610	611	612	613	614	615	616	617	618	619	620	621	622	623	624	625	626	627	628	629	630	631	632	633	634	635	636	637	638	639	640	641	642	643	644	645	646	647	648	649	650	651	652	653	654	655	656	657	658	659	660	661	662	663	664	665	666	667	668	669	670	671	672	673	674	675	676	677	678	679	680	681	682	683	684	685	686	687	688	689	690	691	692	693	694	695	696	697	698	699	700	701	702	703	704	705	706	707	708	709	710	711	712	713	714	715	716	717	718	719	720	721	722	723	724	725	726	727	728	729	730	731	732	733	734	735	736	737	738	739	740	741	742	743	744	745	746	747	748	749	750	751	752	753	754	755	756	757	758	759	760	761	762	763	764	765	766	767	768	769	770	771	772	773	774	775	776	777	778	779	780	781	782	783	784	785	786	787	788	789	790	791	792	793	794	795	796	797	798	799	800	801	802	803	804	805	806	807	808	809	810	811	812	813	814	815	816	817	818	819	820	821	822	823	824	825	826	827	828	829	830	831	832	833	834	835	836	837	838	839	840	841	842	843	844	845	846	847	848	849	850	851	852	853	854	855	856	857	858	859	860	861	862	863	864	865	866	867	868	869	870	871	872	873	874	875	876	877	878	879	880	881	882	883	884	885	886	887	888	889	890	891	892	893	894	895	896	897	898	899	900	901	902	903	904	905	906	907	908	909	910	911	912	913	914	915	916	917	918	919	920	921	922	923	924	925	926	927	928	929	930	931	932	933	934	935	936	937	938	939	940	941	942	943	944	945	946	947	948	949	950	951	952	953	954	955	956	957	958	959	960	961	962	963	964	965	966	967	968	969	970	971	972	973	974	975	976	977	978	979	980	981	982	983	984	985	986	987	988	989	990	991	992	993	994	995	996	997	998	999	1000	1001	1002	1003	1004	1005	1006	1007	1008	1009	1010	1011	1012	1013	1014	1015	1016	1017	1018	1019	1020	1021	1022	1023	1024	1025	1026	1027	1028	1029	1030	1031	1032	1033	1034	1035	1036	1037	1038	1039	1040	1041	1042	1043	1044	1045	1046	1047	1048	1049	1050	1051	1052	1053	1054	1055	1056	1057	1058	1059	1060	1061	1062	1063	1064	1065	1066	1067	1068	1069	1070	1071	1072	1073	1074	1075	1076	1077	1078	1079	1080	1081	1082	1083	1084	1085	1086	1087	1088	1089	1090	1091	1092	1093	1094	1095	1096	1097	1098	1099	1100	1101	1102	1103	1104	1105	1106	1107	1108	1109	1110	1111	1112	1113	1114	1115	1116	1117	1118	1119	1120	1121	1122	1123	1124	1125	1126	1127	1128	1129	1130	1131	1132	1133	1134	1135	1136	1137	1138	1139	1140	1141	1142	1143	1144	1145	1146	1147	1148	1149	1150	1151	1152	1153	1154	1155	1156	1157	1158	1159	1160	1161	1162	1163	1164	1165	1166	1167	1168	1169	1170	1171	1172	1173	1174	1175	1176	1177	1178	1179	1180	1181	1182	1183	1184	1185	1186	1187	1188	1189	1190	1191	1192	1193	1194	1195	1196	1197	1198	1199	1200	1201	1202	1203	1204	1205	1206	1207	1208	1209	1210	1211	1212	1213	1214	1215	1216	1217	1218	1219	1220	1221	1222	1223	1224	1225	1226	1227	1228	1229	1230	1231	1232	1233	1234	1235	1236	1237	1238	1239	1240	1241	1242	1243	1244	1245	1246	1247	1248	1249	1250	1251	1252	1253	1254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# channeling.xlsm program

channeling.xlsm - Microsoft Excel

File Home Insert Page Layout Formulas Data Review View Developer

Clipboard Font Alignment Number Styles Cells Editing

I22 100

1 Calculation of channeling half-angles  
2 enter parameters in yellow cells only

3  
4  
5

6 **Beam**

7

8 atomic number of  $Z_1$  2 He  
9 Energy of projectile  $E$  0.3 MeV

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15 Calculate half-angles and Xmins

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18 axial  $\psi_{1/2}$  1.16 deg  
19 planar  $\psi_{1/2}$  0.32 deg

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21 axial  $\chi$ -min 0.399 w/overlayer  
22 axial  $\chi$ -min 0.035 w/o overlayer  
23 planar  $\chi$ -min 0.286 w/o overlayer

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