


Calculating and Mapping Unintentional Ion Channeling in Polycrystalline Materials*

SAND2016-8024C

**Barney L. Doyle, Paolo Rossi, George Vizkelethy, Khalid M. Hattar,
Daniel C. Bufford, Brittany R. Muntifering, Cajer Gong, Aldo
Corona, Anh Q. Nguyen**

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

*Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000.



We propose here that it is important to include the effect of ion channeling when considering the equivalence of using ions accelerated to high energies to simulate the displacement damage produced by energetic neutrons

- Ions that channel will make less (maybe no) displacement damage.
- The primary knock-on atoms (PKAs) recoiled by neutrons are omnidirectional in the forward direction and of such low energies that they are unlikely to channel
- The monodirectional high energy ions implanted as PKAs will certainly channel if individual crystallites in the material are oriented with their crystallographic axes or planes aligned with the direction of the beam.
- This presentation will ameliorate this uncertainty in ion-neutron equivalence by combining:
 - theoretical calculations of axial and planar channeling $\frac{1}{2}$ angles and dechanneling fractions
 - with orientation distribution measurements of polycrystalline samples performed on the TEM
- We will show how this approach quantitatively determines the probability that accelerated ions will channel in:
 - randomly oriented and
 - textured polycrystalline materials
 - and even map the position on the sample where such ion channeling occurs

Ion channeling is usually thought of as a type of IBA where the Rutherford Backscattering of single crystal samples is measured as a function of tilt angle.

70

B. R. Appleton and G. Foti

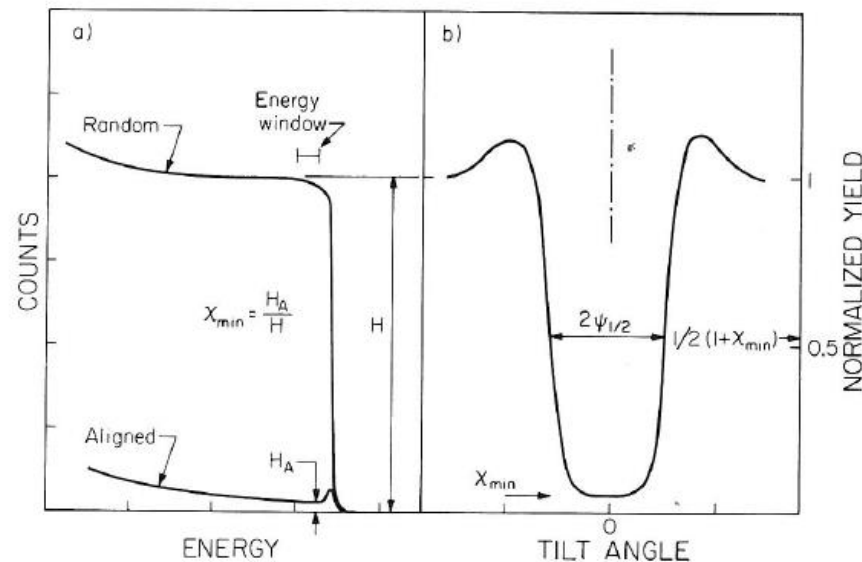


Figure 3.1 Backscattering spectra and angular yield profile.

...but this data also demonstrates that the small impact parameter collisions required for RBS, and the subsequent recoiling of target atoms, is significantly reduced for the channeling condition.

This is the premise of this paper.



Outline

- Parameterizing the physics of ion channeling
- Representing axial and planar ion channeling as “equal angle projections”
- Calculating channeling probabilities for randomly oriented polycrystalline materials
- Including the effects of texture
 - crystallite orientation measurements
 - incorporating this data with equal angle projections
 - calculating channeling probability
 - mapping where ion channeling will occur
- Experiments

Parameterizing Channeling

- A paper was written last year that detailed the calculation of RBS axial and planar channeling $\frac{1}{2}$ angles and minimum yields for all ions at all energies on all bcc, fcc and diamond lattice crystals.
- This paper parameterized all of the charts generated by John Barrett (Phys. Rev. B3 (1973) 1782) used to improve the famous channeling theory of Jens Lindhard, Mat.-Fys. Medd, 34 (1965) 1.)



Parameterization of ion channeling half-angles and minimum yields ☆

Barney L. Doyle

Radiation Solid Interactions Department 01111, Sandia National Laboratories, P.O. Box 5800, Albuquerque, NM 87185-MS1056, United States

ARTICLE INFO

Article history:
Received 10 July 2015
Received in revised form 19 August 2015
Accepted 20 August 2015
Available online xxxx

Keywords:
Ion channeling
Half-angles
Minimum yields

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 $\langle uvr \rangle$ axes and $\{hkl\}$ planes up to $\{555\}$. The program is open source and available at <http://www.sandia.gov/pcnsc/departments/iba/ibatable.html>.

© 2015 Elsevier B.V. All rights reserved.

- The paper above describes an Excel program that makes this calculation of channeling parameters quite easy. The program can be found at:

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

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 atomic number of Z_1 2 He
8 Energy of projectil E 0.3 MeV

9

10

11

12

13

14

15 Calculate half-angles and Xmins

16

17

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

20

21 axial χ -min 0.399 w/overlayer
22 axial χ -min 0.035 w/o overlayer
23 planar χ -min 0.286 w/o overlayer

24

25

26

27

28

29

30

31

32

33

34

35

36

37

38

39

40

41

42

43

44

45

46

47

48

49

50

51

52

53

54

55

56

57

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

1255

1256

1257

1258

1259

1260

1261

1262

1263

1264

1265

1266

1267

1268

1269

1270

1271

1272

1273

1274

1275

1276

1277

1278

1279

1280

1281

1282

1283

1284

1285

1286

1287

1288

1289

1290

1291

1292

1293

1294

1295

1296

1297

1298

1299

1300

1301

1302

1303

1304

1305

1306

1307

1308

1309

1310

1311

1312

1313

1314

1315

1316

1317

1318

1319

1320

1321

1322

1323

1324



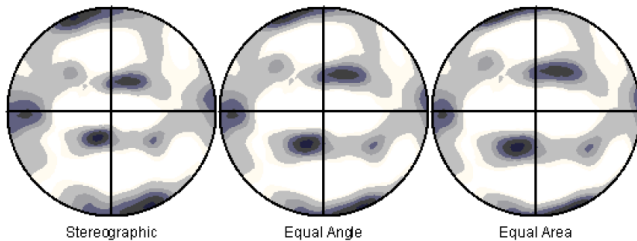
Outline

- Parameterizing the physics of ion channeling
- Representing axial and planar ion channeling as “equal angle projections”
- Calculating channeling probabilities for randomly oriented polycrystalline materials
- Including the effects of texture
 - crystallite orientation measurements
 - incorporating this data with equal angle projections
 - calculating channeling probability
 - mapping where ion channeling will occur
- Experiments

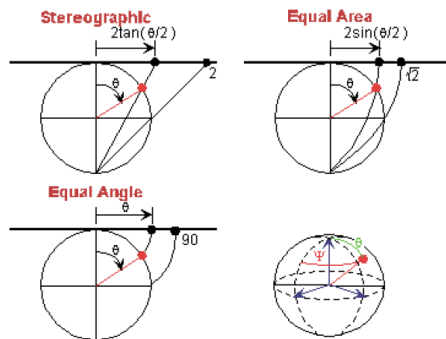
Equal Angle Projections are commonly used for displaying texture, but here we show how projecting plots of axial and planar channeling is also benefitted by this type of projection

Projection (Stereographic, Equal Area, Equal Angle)

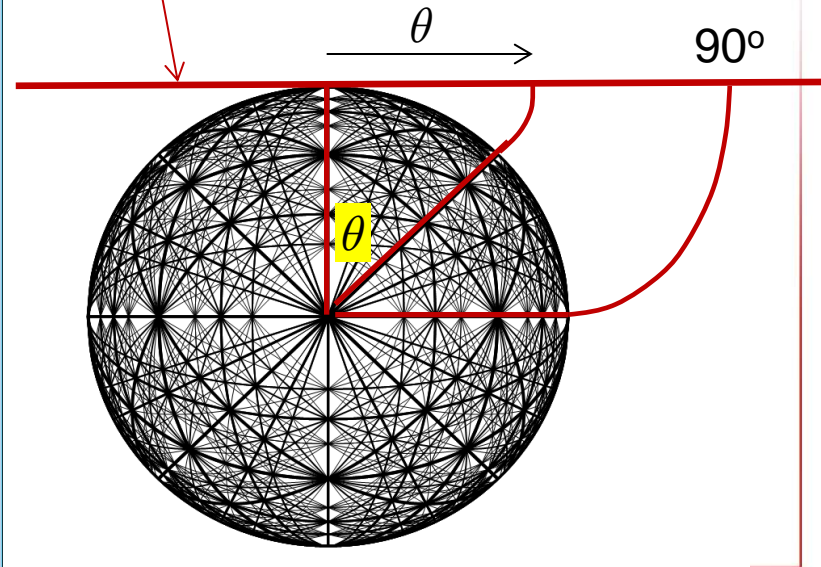
In pole figures, inverse pole figures and Axis/Angle MDF sections three different methods for plotting the 2-dimensional projections of the 3-dimensional orientation data are available. The projections types include stereographic, equal area and equal angle. The Equal Angle is not a true projection method but a simple mapping that is sometimes used. The Stereographic projection expands any features near the outside edges of the plot; whereas, the Equal Area projection expands detail at the center of the plot. Examples of the different types are shown below for a (111) intensity pole figure.



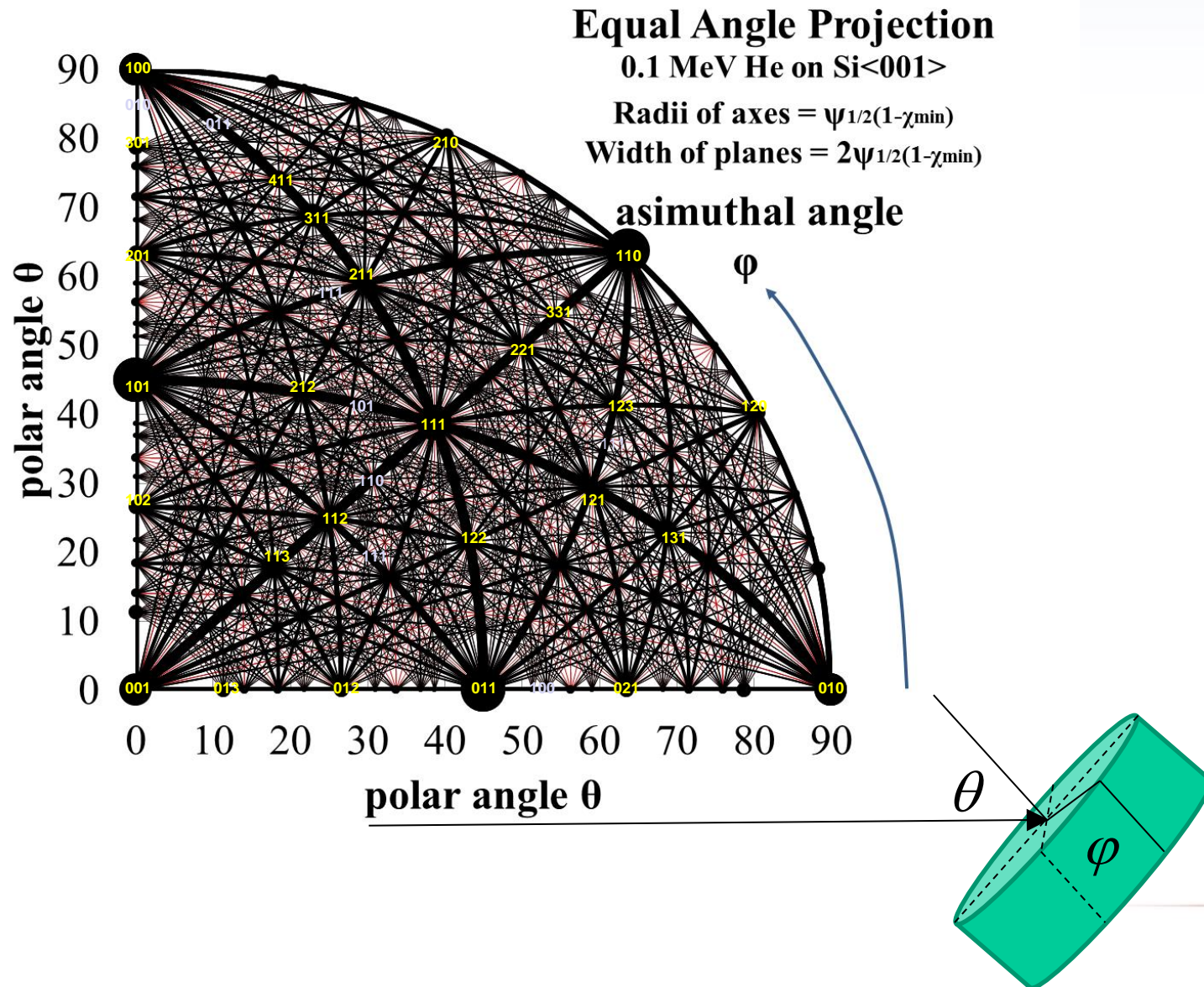
A schematic of the projection methods is shown below:



By projecting channeling onto this plane this way, axes can be plotted as circles with a radius of $\Psi_{1/2}^a$, and planes as lines of constant width $2\Psi_{1/2}^p$.



Geometry used to represent ion channeling



1.7 MeV Au on Au channeling half angles

axial channeling		1/2 angles	
e ²		1.44E-05	MeV-A
atomic number of projectile	Z ₁	79	Au
atomic # of target	Z ₂	79	Au
atomic weight of target	M2	196.9665	amu
Energy of projectile	E	1.7	MeV
conventional cell size	cc	4.078	Ang
lattice		fcc	
lattice type		1	u
Miller indeces		111	1
axis lattice factor	fa	1.73	loo
lattice spacing	d	7.06330319	Ang
Following the EQUATIONSL FOR CHANNELING in the IBA Handbook, p645			
		0.4685*C6^(1/3)	
thomas fermi screening length	a	0.10918607	Ang
Debye Temp	theat-D	170	K
Room Temp	T	293	K
x"=Theta-D/T	x"	0.58020478	
debye fn	phi-D	0.8737759	
rms thermal amplitude	u1	0.08762425	Ang
characteristic axial channeling angle	Ψ ₁	6.99901754	deg
		0.1221469	rad
ratio of a to d	a/d	0.01096125	
parameter to use in Frs	x'	1.35811809	
adimentional axial channeling Fn	Frs	0.71301132	
channeling 1/2 angle for Ψ ₁ <a/d	Ψ _{1/2}	4.34162952	deg
channeling 1/2 angle for Ψ ₁ >a/d	Ψ _{1/2}	2.09673967	deg
channeling 1/2 angle to use	Ψ _{1/2}	2.10	deg

planar channeling			
atomic number of projectile	Z ₁	79	
atomic # of target	Z ₂	79	
atomic weight of target	M2	196.9665	
Energy of projectile	E	1.7	MeV
conventional cell size	cc	4.078	Ang
lattice		fcc	
lattice type		1	h
Miller indeces		11	0
plane lattice factor	f' or fp	0.35355339	
avg atomic spacing between planes	dp	1.44179073	Ang
density	rho	19.3	g/cm3
Avagodros number	Nav	6.02E+23	at/mole
target atoms/cm3	N	5.9017E+22	atoms/cm3
		0.05901709	atoms/A3
characteristic planer channeling angle	Ψ _a	2.68E+00	deg
Fps parameters			
	x'	1.81082411	
	y'	18.6223376	
adimentional planar channeling function	Fps	0.82413568	
Planar channeling 1/2 angle	Ψ _{1/2}	1.44	deg

Equal Angle Projection - axes

To plot solid circles at position (x,y) to represent an (h,k,l) channeling axes:

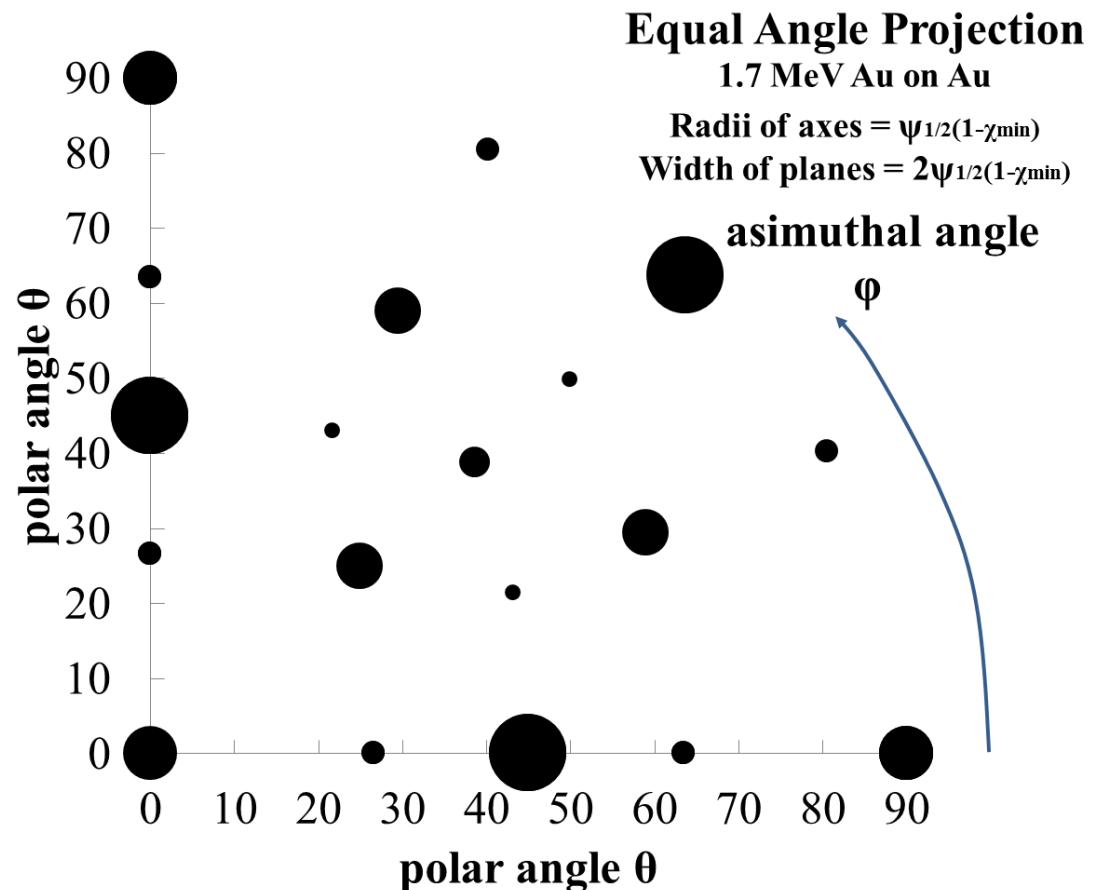
$$1. \text{radius} = \Psi_{1/2}^{a-hkl} (1 - \chi_{\min})$$

$$2. \theta = \cos^{-1}(l / (h^2 + k^2 + l^2)^{1/2})$$

$$3. \varphi = \tan^{-1}(k / l)$$

$$4. x = \theta \cos(\varphi)$$

$$5. y = \theta \sin(\varphi)$$



equal angle projection of planes

first parameterize circle representing plane

for standard Miller indices h, k, l

The normal to this plane is defined by:

$$n_z = l / (h^2 + k^2 + l^2)^{1/2}, n_y = k / (h^2 + k^2 + l^2)^{1/2}, n_x = h / (h^2 + k^2 + l^2)^{1/2}$$

or

$$\hat{n} = \begin{pmatrix} \cos(\varphi_n) \sin(\theta_n) \\ \sin(\theta_n) \sin(\varphi_n) \\ \cos(\theta_n) \end{pmatrix}$$

$$\theta_n = \cos^{-1}(n_z)$$

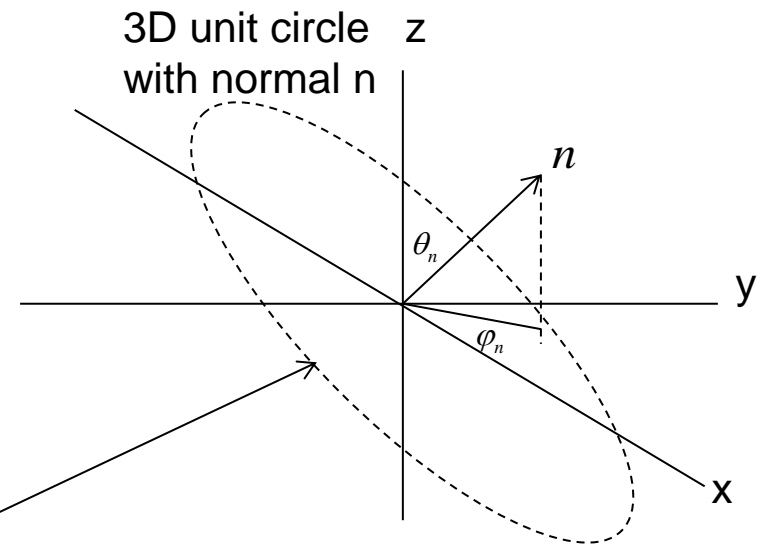
$$\varphi_n = \tan^{-1}(k / l)$$

The vector \hat{u} is defined as:

$$\hat{u} = \begin{pmatrix} -\sin(\varphi_n) \\ \cos(\varphi_n) \\ 0 \end{pmatrix} \text{ and then } \hat{n} \times \hat{u} = \begin{pmatrix} \cos(\theta_n) \cos(\varphi_n) \\ \cos(\theta_n) \sin(\varphi_n) \\ -\sin(\theta_n) \end{pmatrix}$$

The parametric form of a 3D unit circle with normal \hat{n} is:

$$\vec{P}(t) = \cos(t)\hat{u} + \sin(t)\hat{n} \times \hat{u}$$



equal angle projection of planes

Then project this circle using equal angle projection

for a set of t values $\{t\}$ calculate the $P_x(t), P_y(t), P_z(t)$

using:

$$1. \vec{P}(t) = \cos(t)\hat{u} + \sin(t)\hat{n} \times \hat{u}$$

The equal angle projection is then made by calculating $x(t)$ and $y(t)$

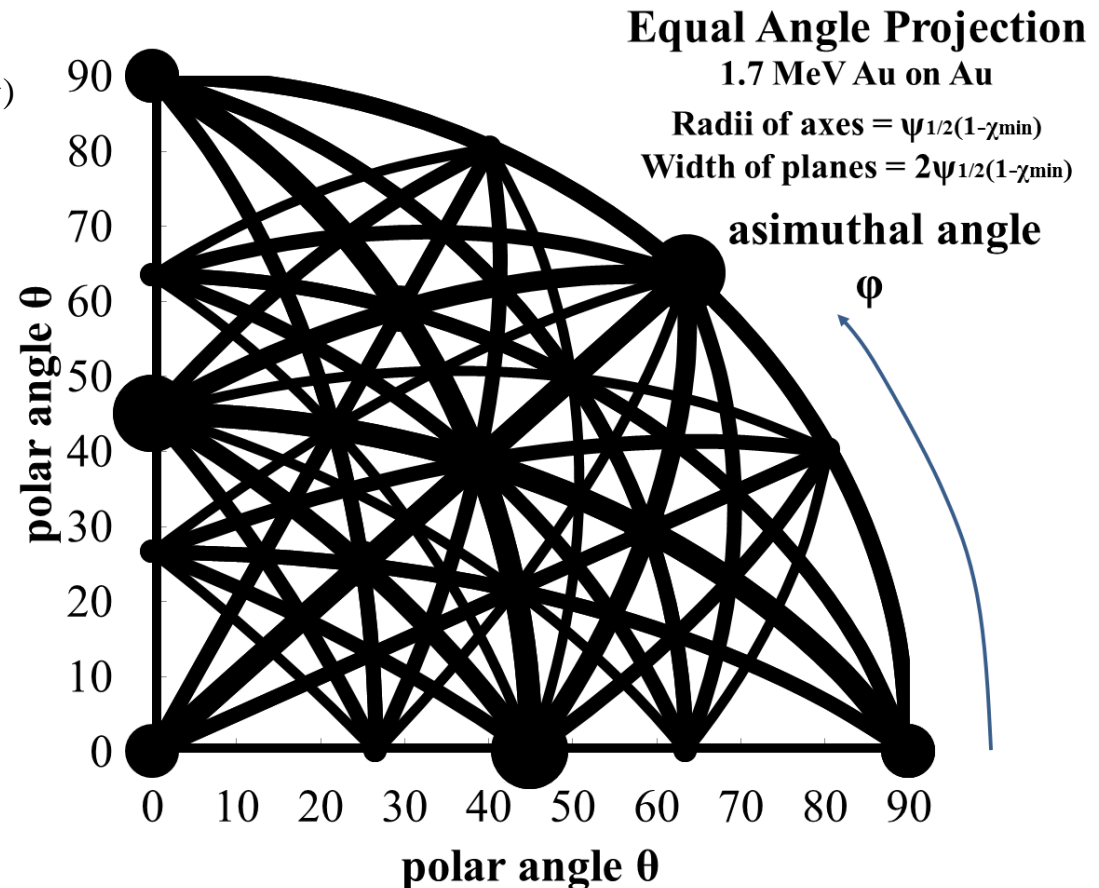
$$2. \theta(t) = \cos^{-1}(P_z / (P_x(t)^2 + P_y(t)^2 + P_z(t)^2)^{1/2})$$

$$3. \varphi(t) = \tan^{-1}(P_y(t) / P_x(t))$$

$$4. x(t) = \theta(t) \cos(\varphi(t))$$

$$5. y(t) = \theta(t) \sin(\varphi(t))$$

6. the set of $(x(t), y(t))$ points are plotted and connected with a line of width $= \Psi_{1/2}^{p-hkl} (1 - \chi_{\min})$



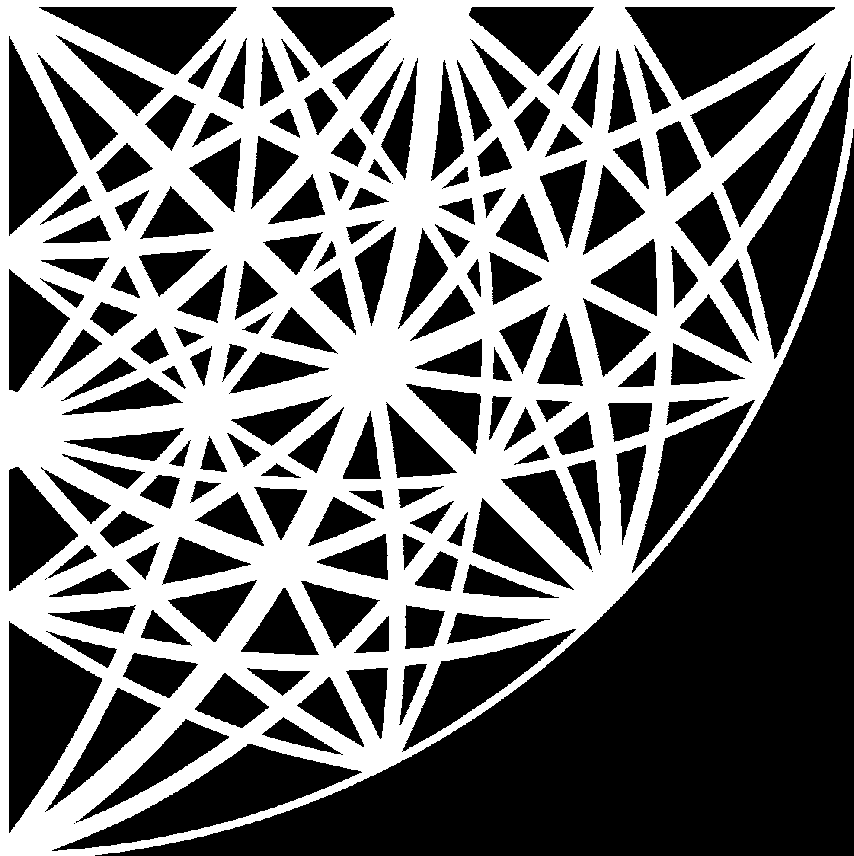


Outline

- Parameterizing the physics of ion channeling
- Representing axial and planar ion channeling as “equal angle projections”
- **Calculating channeling probabilities for randomly oriented polycrystalline materials**
- Including the effects of texture
 - crystallite orientation measurements
 - incorporating this data with equal angle projections
 - calculating channeling probability
 - mapping where ion channeling will occur
- Experiments

to calculate the channeling probability for randomly oriented polycrystalline materials:

1. the equal angle projections plotted in excel are saved as bitmap files.
2. then read into a 2D array of 1's and 0's
3. in plot below white areas are 1's and indicate channeling, black areas are 0's and indicate dechanneling
4. this quadrant of equal angle space has a 1136 cell radius
5. the channeling probability is then the sum of all the 1's in this region divided by $3.14 * 1136^2 / 4$ which is 57%



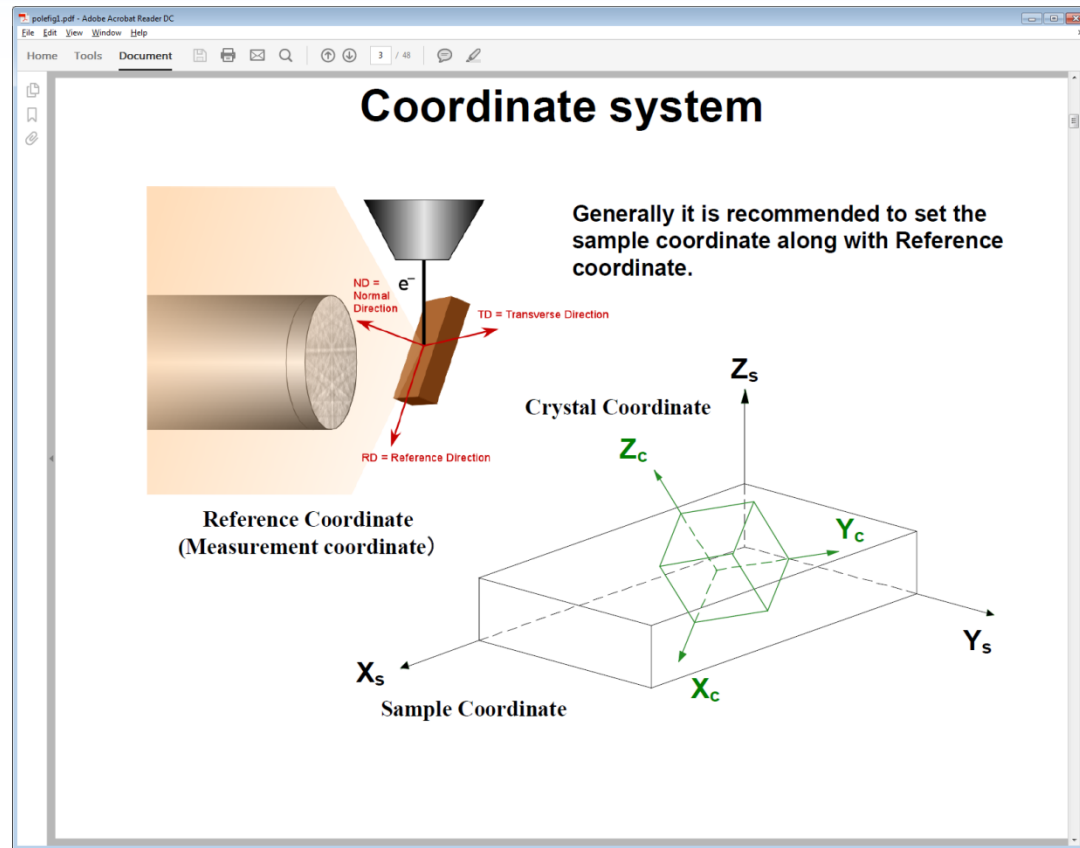
sum=	574892
total=	1013552
C-Prob	0.5672



Outline

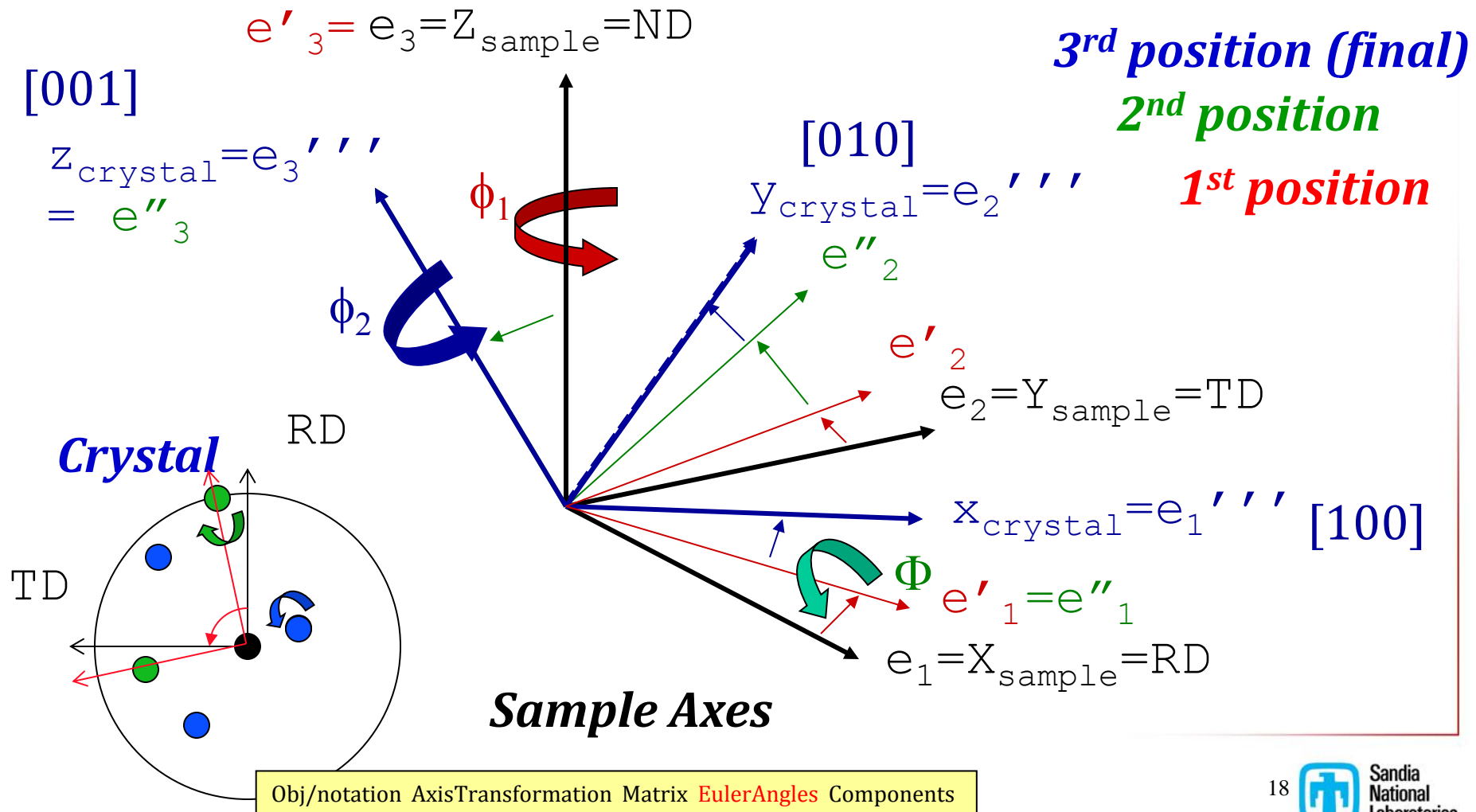
- Parameterizing the physics of ion channeling
- Representing axial and planar ion channeling as “equal angle projections”
- Calculating channeling probabilities for randomly oriented polycrystalline materials
- **Including the effects of texture**
 - crystallite orientation measurements
 - incorporating this data with equal angle projections
 - calculating channeling probability
 - mapping where ion channeling will occur
- Experiments

Definitions of Sample, Crystallite and Reference-Measurement coordinate systems for EBSD or Precession TEM



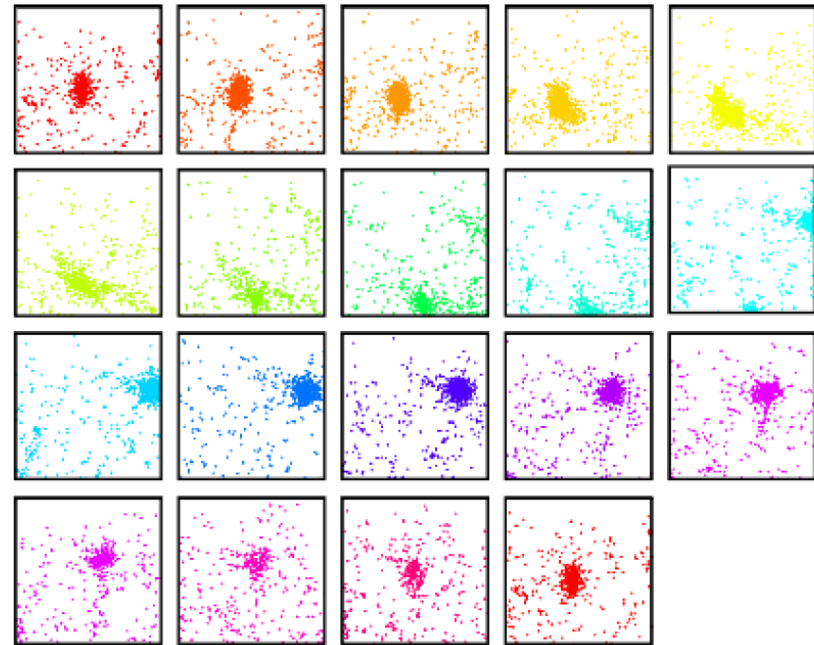
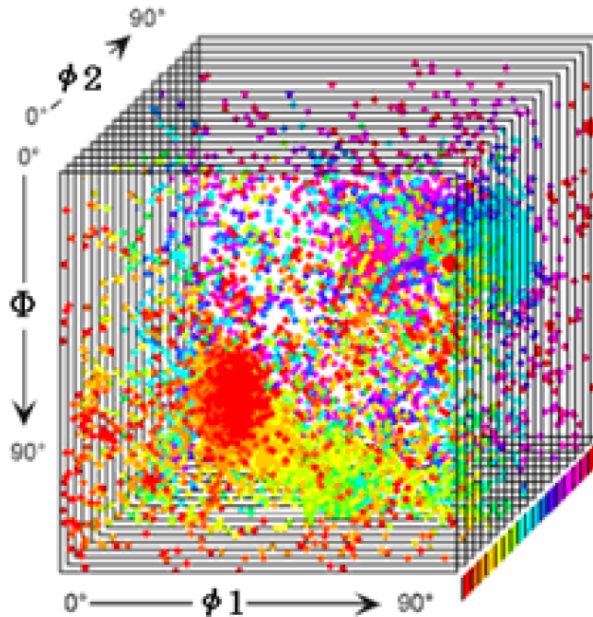
As the e-beam scans across the sample it scatters producing Kikuchi bands for EBSD and diffraction spots for Precession TEM yielding the standard Euler angles ($\varphi_1, \Phi, \varphi_2$) of each polycrystal's orientation

Euler Angles, Animated



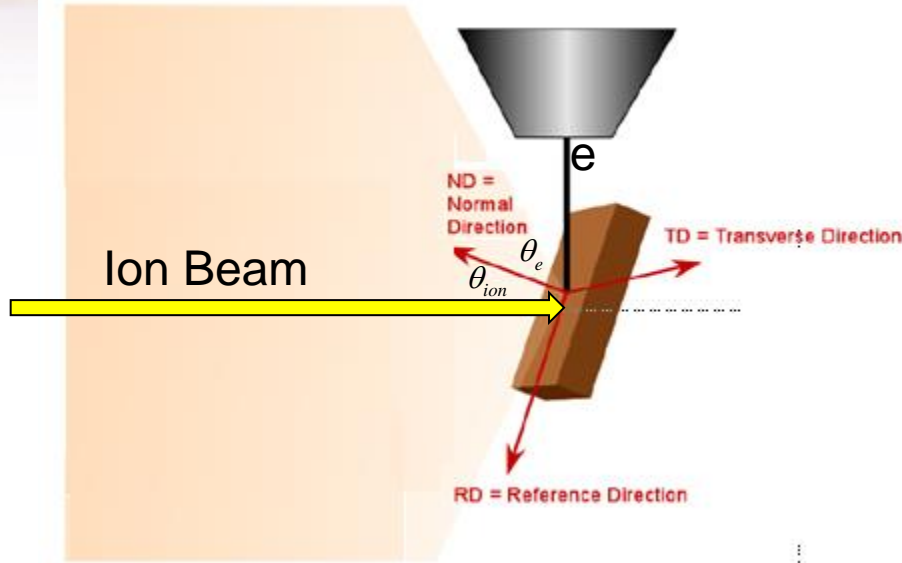
Euler Space Sections

For orientation presentation, it is possible to plot Euler angle (ϕ_1 , Φ , ϕ_2) directly. It is generally said as ODF (Orientation Distribution Function).



In Precession TEM, a diffraction pattern is measured for each scanned position of the beam and the three standard Euler angles (ϕ_1 , Φ , ϕ_2) recorded. The sample is usually perpendicular to the electron beam.

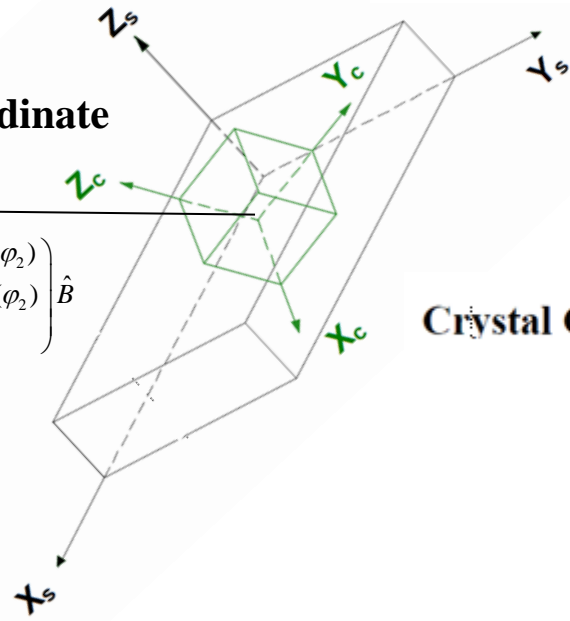
At Sandia the ion beam is perpendicular to the TEM beam, and therefore samples must be tilted. The direction of the ion beam must then be transformed into the coordinate system of each polycrystal to see if channeling occurs.



Ion Beam Coordinate

$\hat{\mathbf{B}}$

Sample Coordinate



Crystal Coordinate

$$\hat{\mathbf{B}}' = \begin{pmatrix} \cos(\varphi_1)\cos(\varphi_2) - \cos(\Phi)\sin(\varphi_1)\sin(\varphi_2) & \cos(\varphi_2)\sin(\varphi_1) + \cos(\Phi)\cos(\varphi_1)\sin(\varphi_2) & \sin(\Phi)\sin(\varphi_2) \\ -\cos(\Phi)\cos(\varphi_2)\sin(\varphi_1) - \cos(\varphi_1)\sin(\varphi_2) & \cos(\Phi)\cos(\varphi_2)\cos(\varphi_1) - \sin(\varphi_1)\sin(\varphi_2) & \sin(\Phi)\cos(\varphi_2) \\ \sin(\Phi)\sin(\varphi_1) & -\sin(\Phi)\cos(\varphi_1) & \cos(\Phi) \end{pmatrix} \hat{\mathbf{B}}$$

The θ and φ orientation of each polycrystallite with respect to the ion beam reference coordinate system is given by:

$$\theta = \cos^{-1}(\hat{B}_z')$$

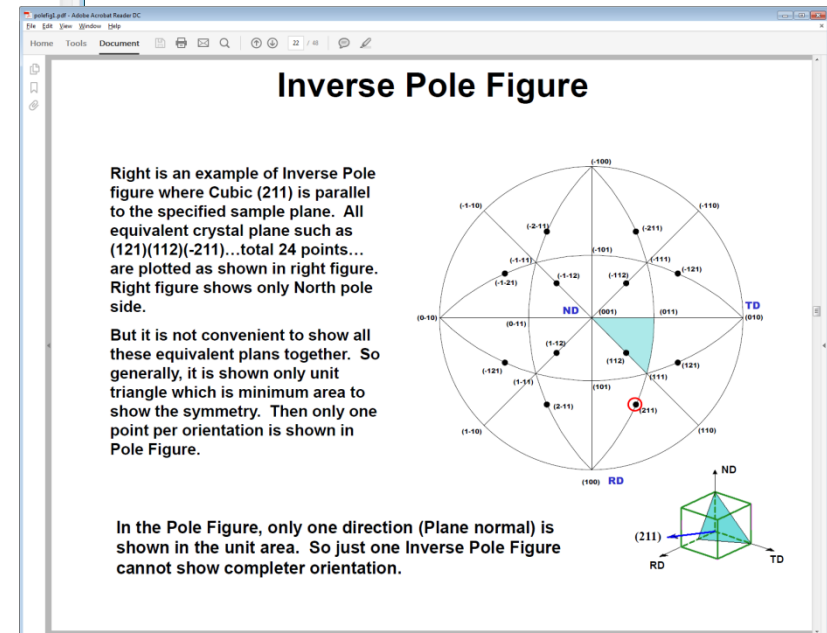
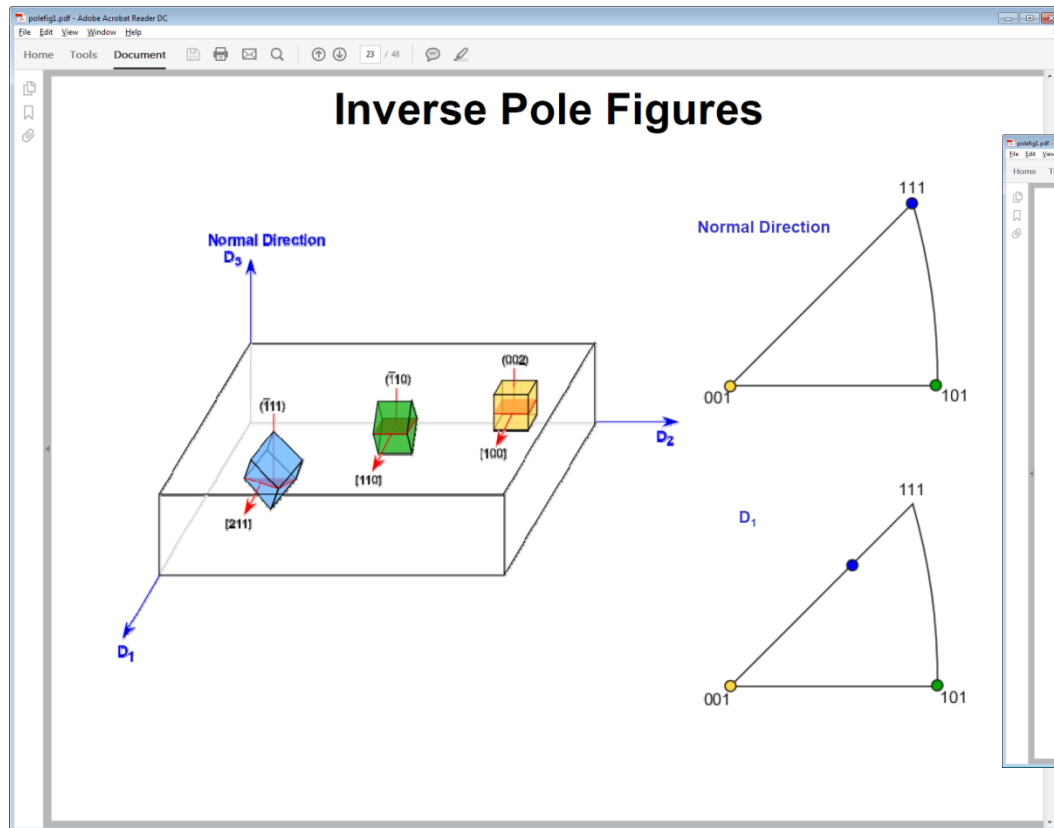
$$\varphi = \tan^{-1}(\hat{B}_y' / \hat{B}_x')$$

and then plotted as (x,y) dots using the equal angle projection:

$$x = \theta \cos(\varphi)$$

$$y = \theta \sin(\varphi)$$

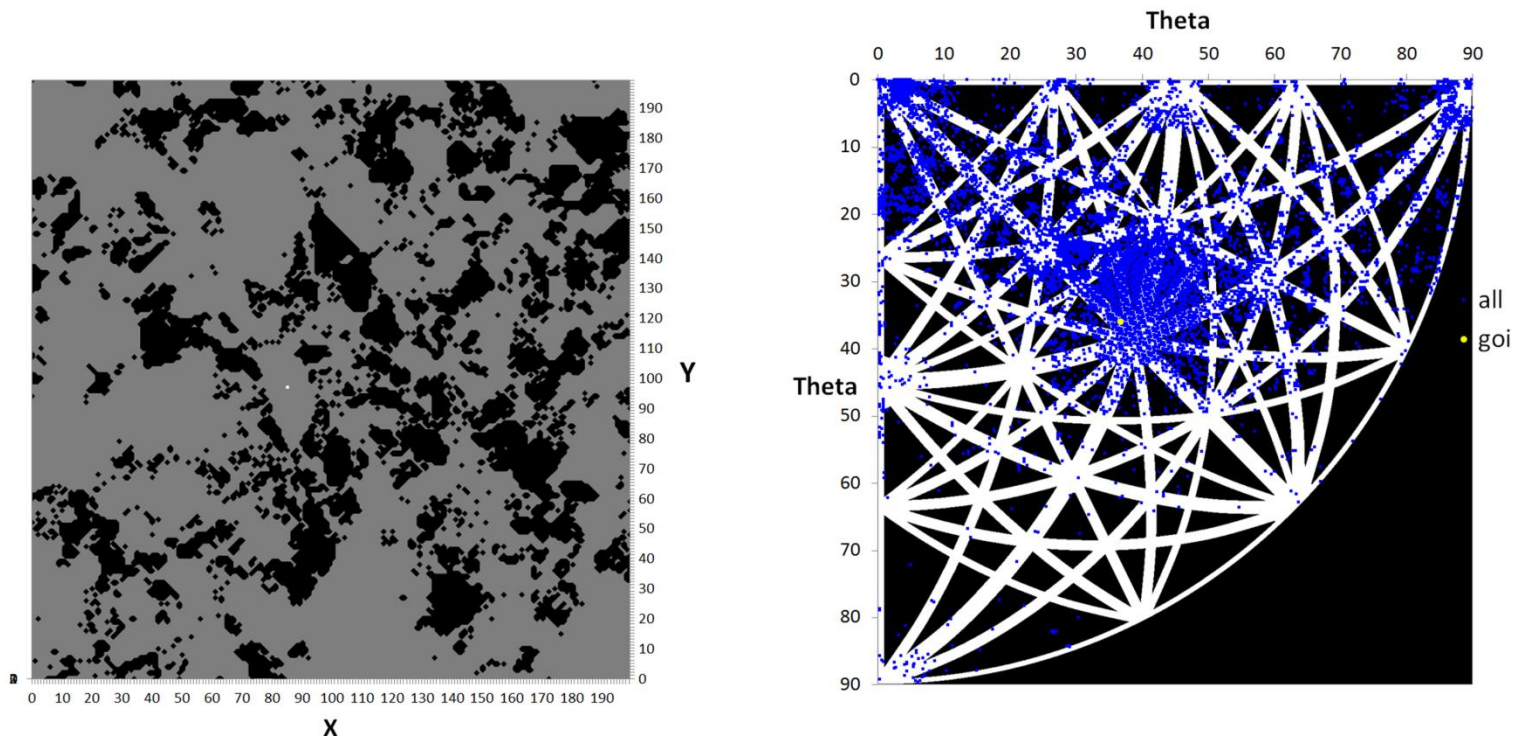
This results in discrete “Ion Beam Direction” inverse pole figures (IPF) being made from the rotated-sample($\varphi_1, \Phi, \varphi_2$) orientation distributions measured by the TEM



1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles ($\varphi_1, \Phi, \varphi_2$) for each polycrystal in the sample are recorded as a function of the (x,y) position of the electron beam.

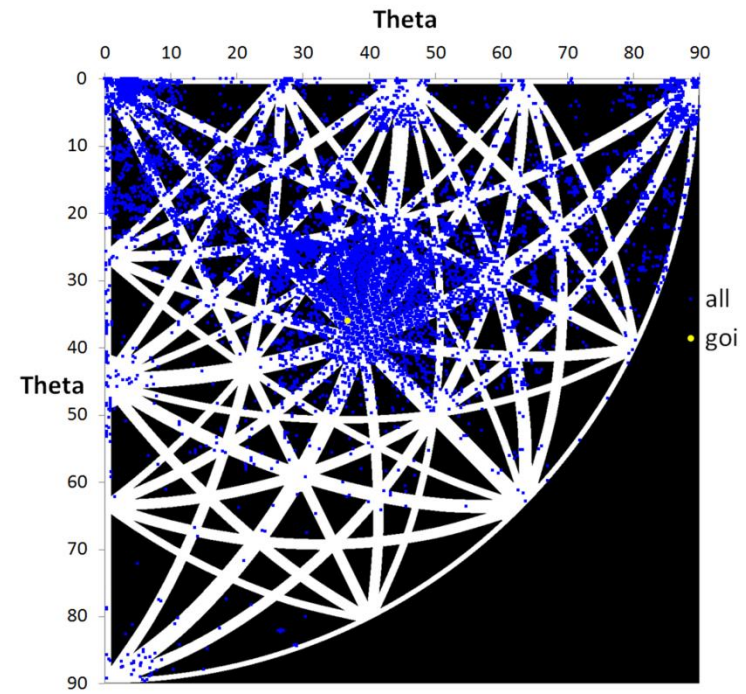
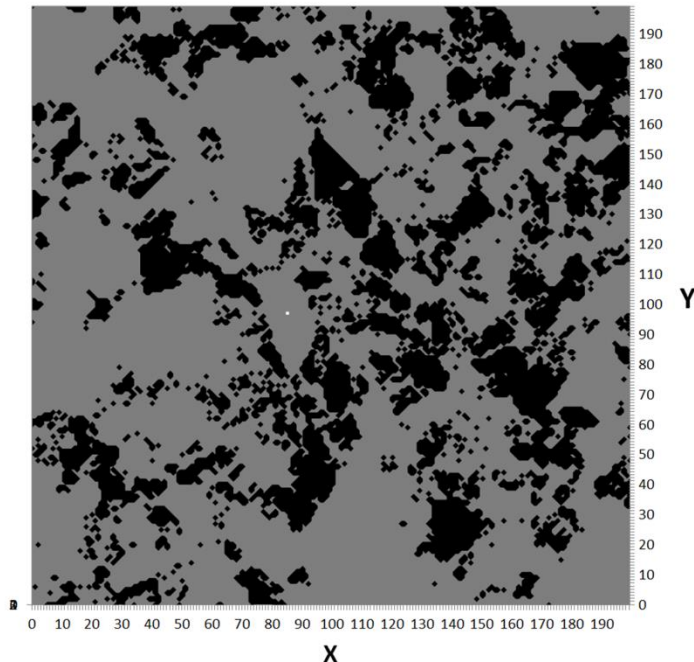
In the figure to the right, an equal angle plot of the discrete 001 IPF (i.e. for a sample not tilted) is plotted over the equal-angle projection of axial and planar channeling. If one of the discrete points corresponds to a white region, the theory contends that channeling will occur.



1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ for each polycrystal in the sample are recorded as a function of the (x, y) position of the electron beam.

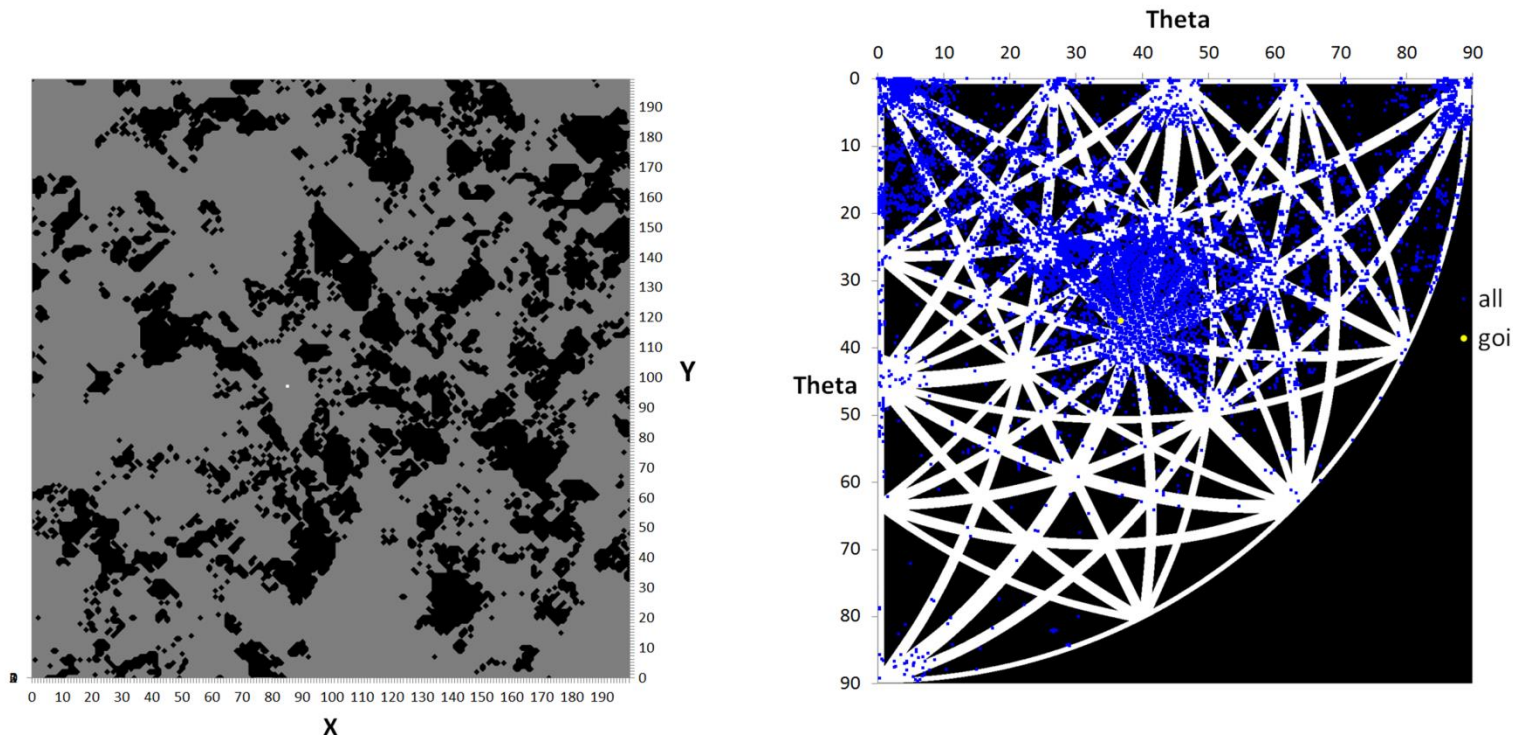
The figure to the left records the position of the beam and points are plotted gray if their corresponding discrete IPF point is in a white channeled region of the plot to the right. For example, the yellow grain of interest (goi) point in the right figure indicates channeling, and the white point in the left figure shows where that grain is.



1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ for each polycrystal in the sample are recorded as a function of the (x, y) position of the electron beam.

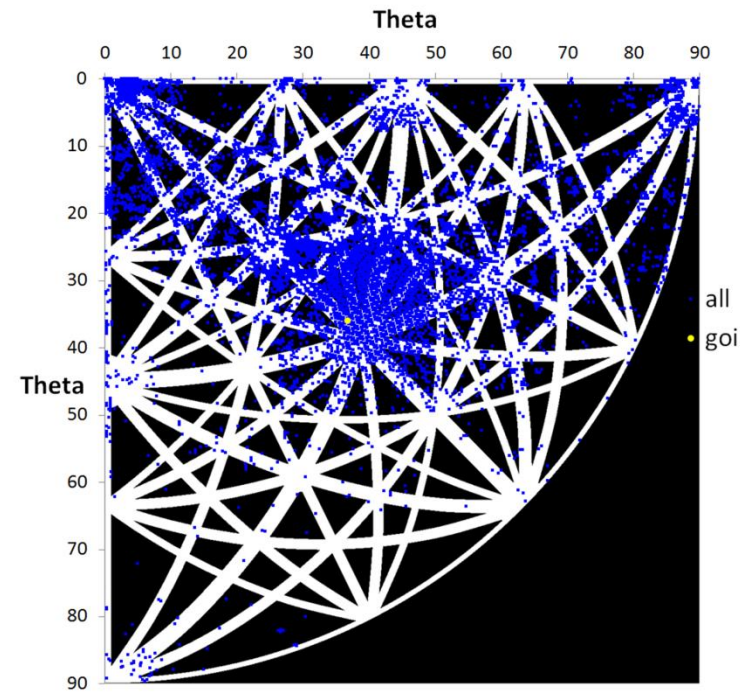
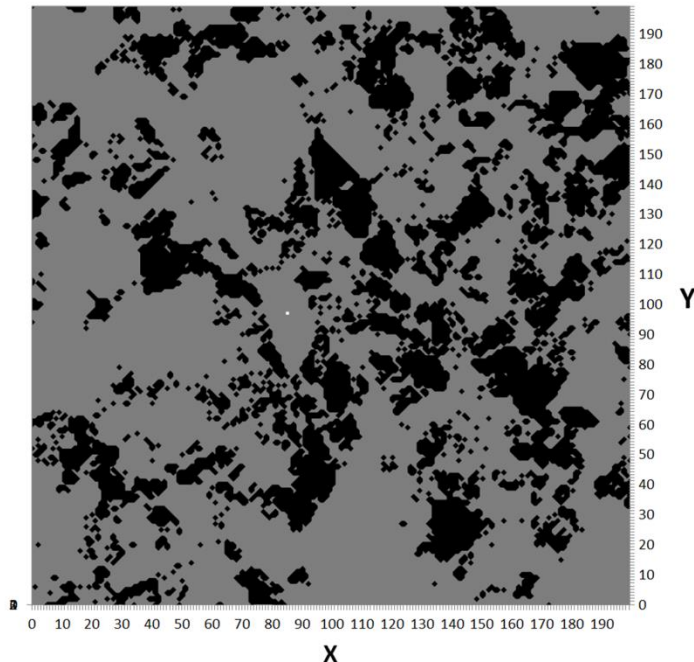
The probability of channeling is determined by counting the number of discrete IPF points that are within the axial or planar channeling half angles (i.e. the white regions of the equal angle projected IPF plots), or just the fractional area of the gray regions on the left figure.



1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles ($\varphi_1, \Phi, \varphi_2$) for each polycrystal in the sample are recorded as a function of the (x,y) position of the electron beam.

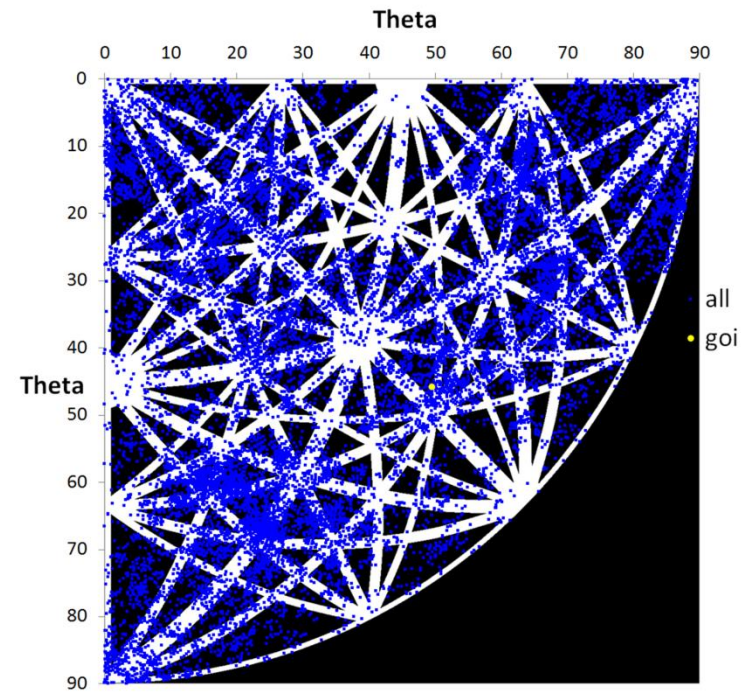
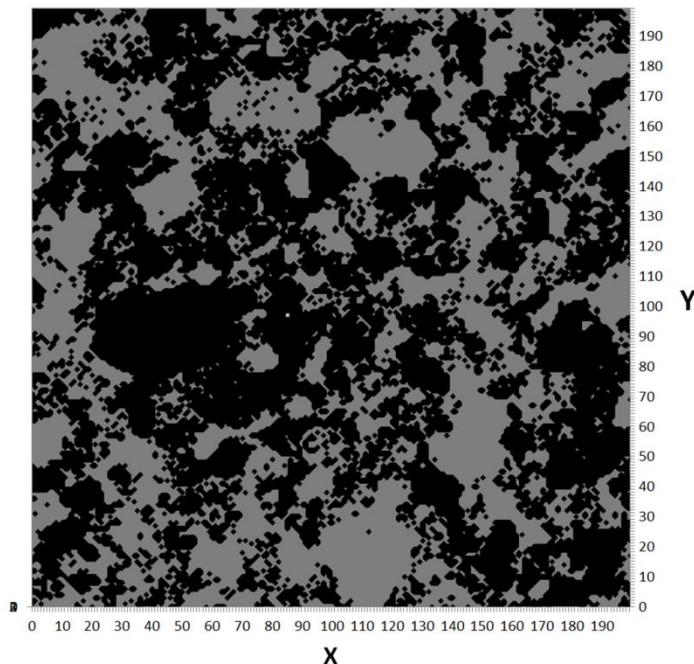
The discrete 001 IPF of this sample clearly shows strong 111 texture, and for this untilted case, the ion beam would have to come in parallel to the electron beam. The channeling probability would be 79% which is higher than the 57% channeling calculated earlier for randomly oriented Au.



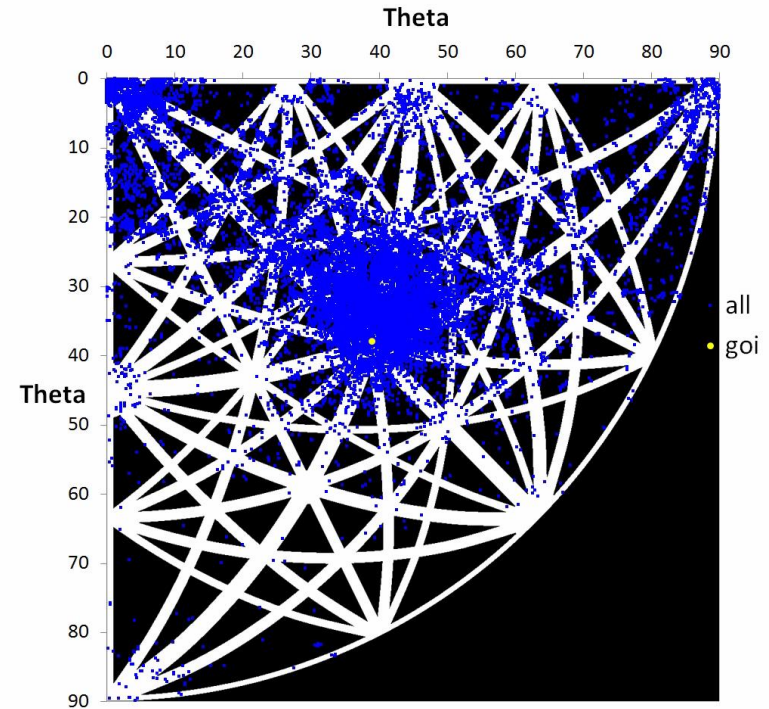
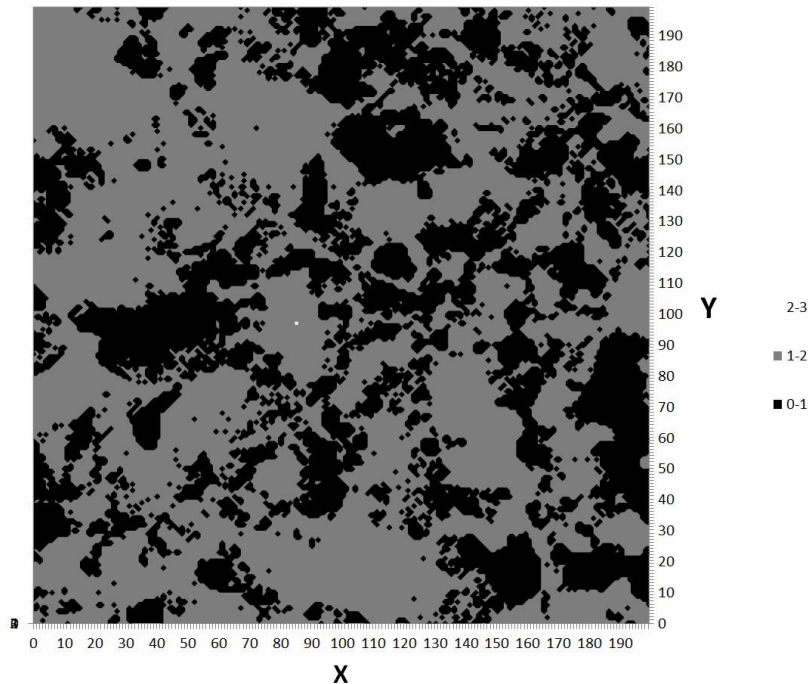
1.7 MeV Au exposure and Precession TEM of polycrystalline Au

The three Euler angles $(\varphi_1, \Phi, \varphi_2)$ for each polycrystal in the sample are recorded as a function of the (x, y) position of the electron beam.

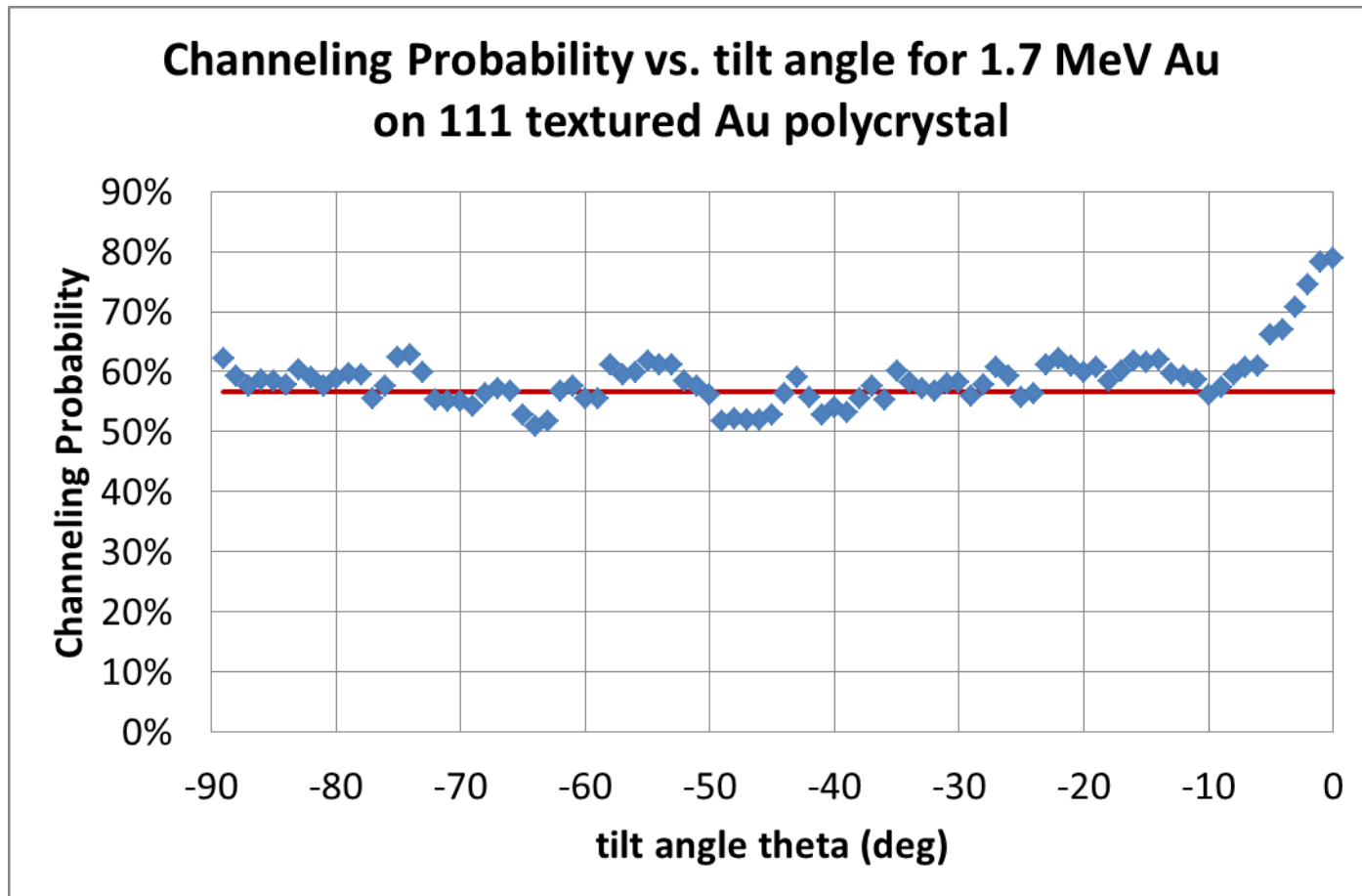
Of course our ion beam can't have the same direction as the TEM beam, and in fact the stage is limited to a $\pm 30^\circ$ rotation. This means that the tilt of the sample in the Beam system is 60° , and the Beam-IPF and corresponding channeling map are plotted below. Here the channeling probability is 57%, which is the same as random. Note that here the goi is not channeling.



equal-angle Beam-IPF of poly Au with 1.7 MeV Au channeling for different tilts



For this sample just about any tilt results in the channeling probability being \sim same as for random



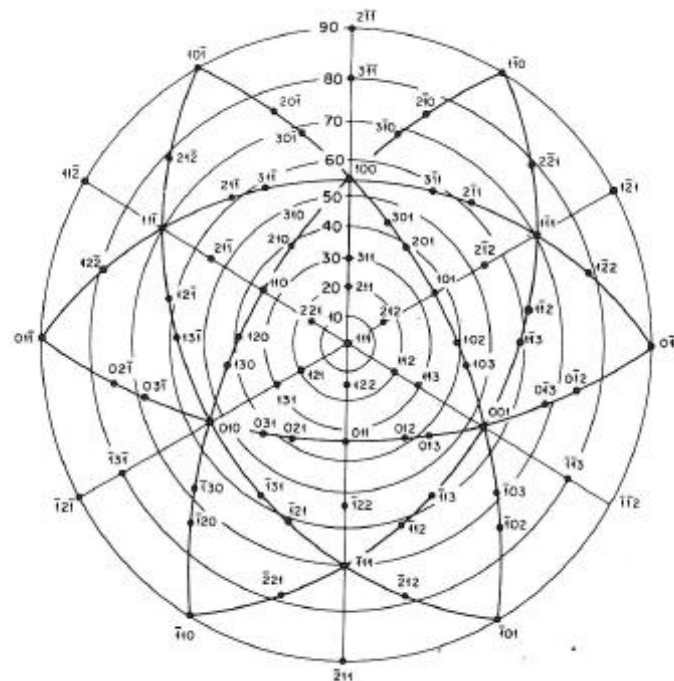
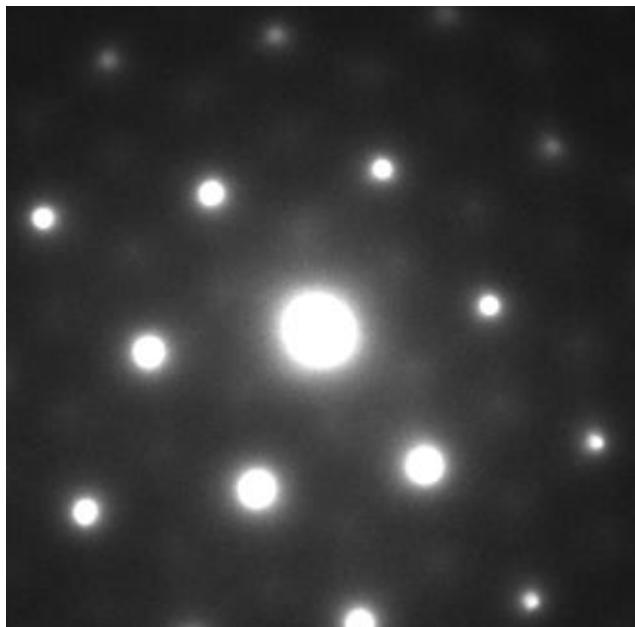


Outline

- Parameterizing the physics of ion channeling
- Representing axial and planar ion channeling as “equal angle projections”
- Calculating channeling probabilities for randomly oriented polycrystalline materials
- Including the effects of texture
 - crystallite orientation measurements
 - incorporating this data with equal angle projections
 - calculating channeling probability
 - mapping where ion channeling will occur
- **Experiments**

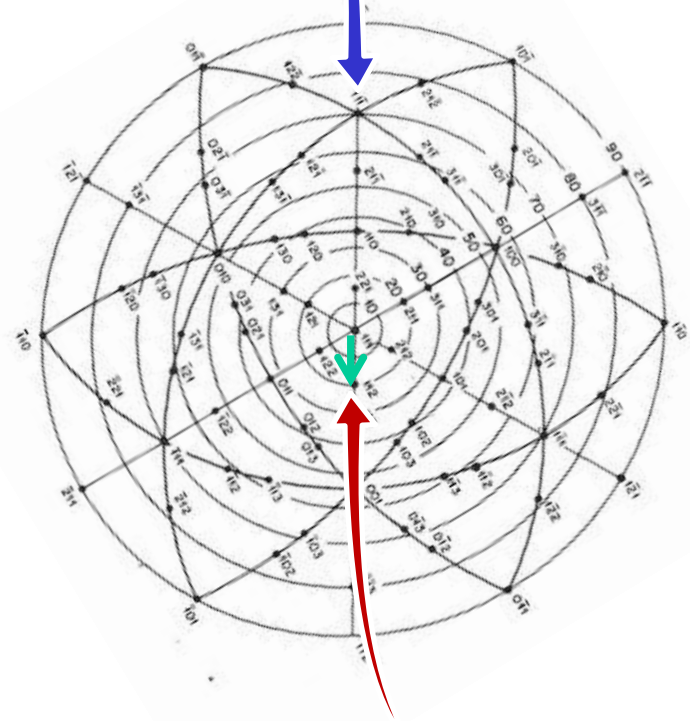
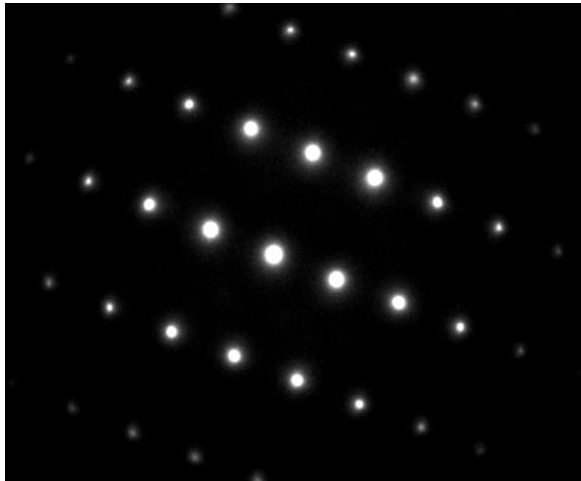
Process to find 111 axial channel for ions

1. precisely position one grain's 111 axis to be parallel with TEM beam using diffraction pattern
2. rotate sample so tilt will follow $1\bar{1}0$ plane toward 112 axis



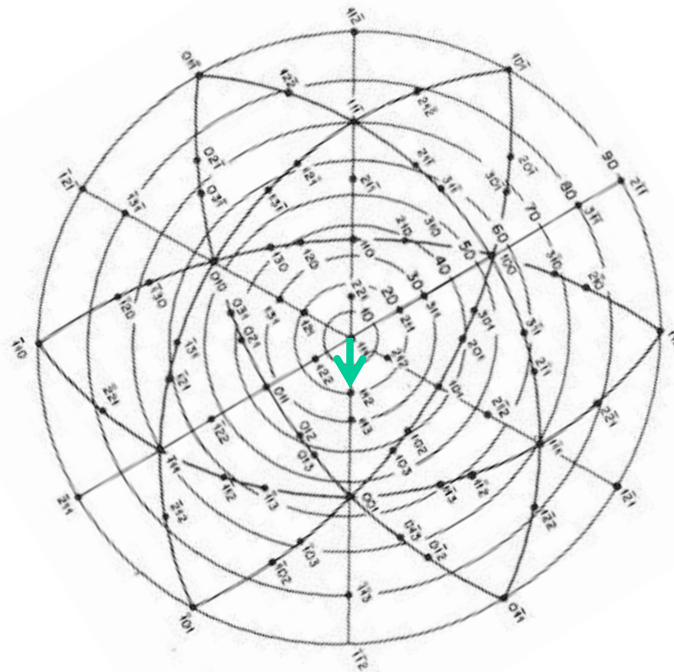
3. the sample is then tilted -19.47 from 0 degrees

- which orients the sample for electrons aligned with the 112 axis (as seen in the diffraction pattern).
- and ion channeling along the 11-1 axis



4. the sample is then implanted with the 1.7 MeV Au to a predetermined fluence.

- It is thought that the grain that has been aligned for channeling will suffer less displacement damage from nearby grains that are not so aligned.

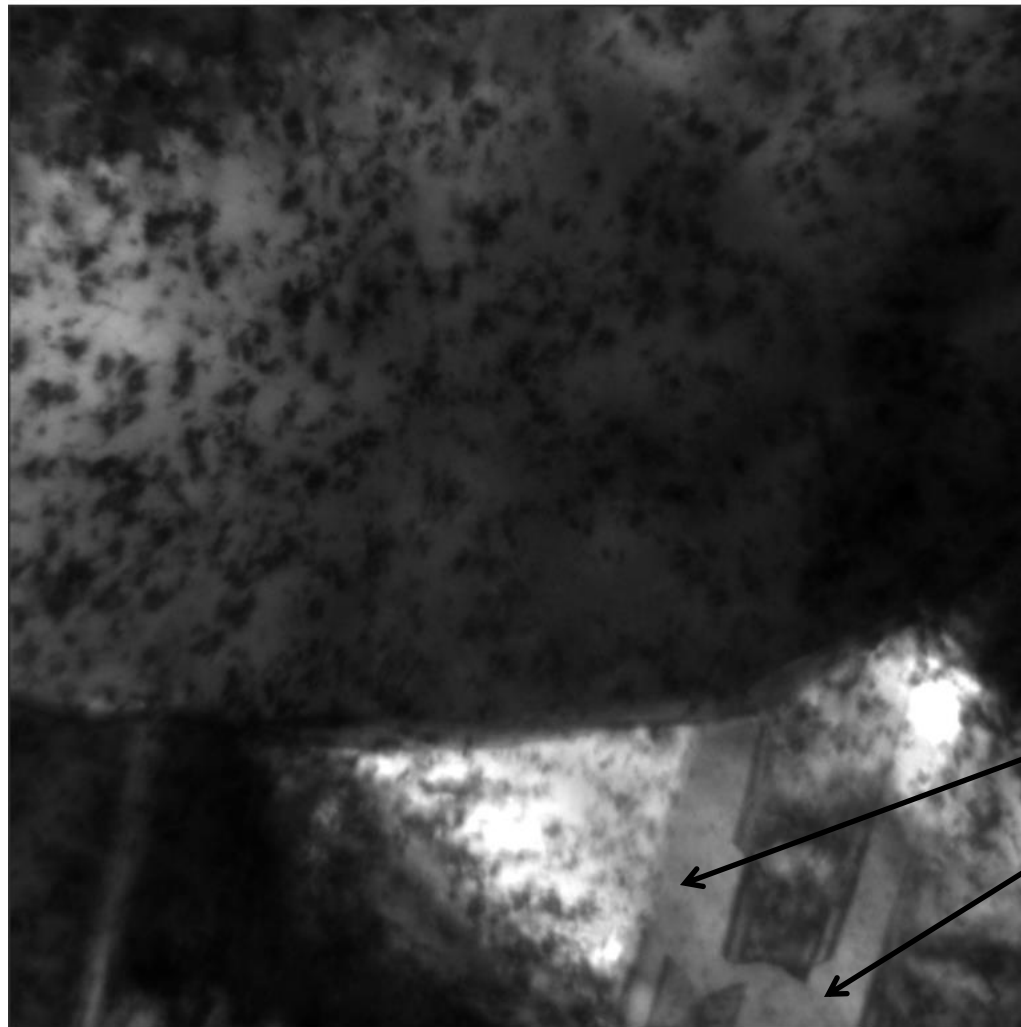


5. The TEM is then used to look for defects like SETs and determine their density

- It is thought that the grain that has been aligned will have a lower density of SFTs, maybe 0.
- Neighboring grains that don't ion channel should have the highest density of SFTs.




Ion current was probably too high, as the damage seen below occurred in only about 10 seconds and is difficult to quantify differences between grains. However, there is no obvious difference between the oriented grain and the other grains in the sample



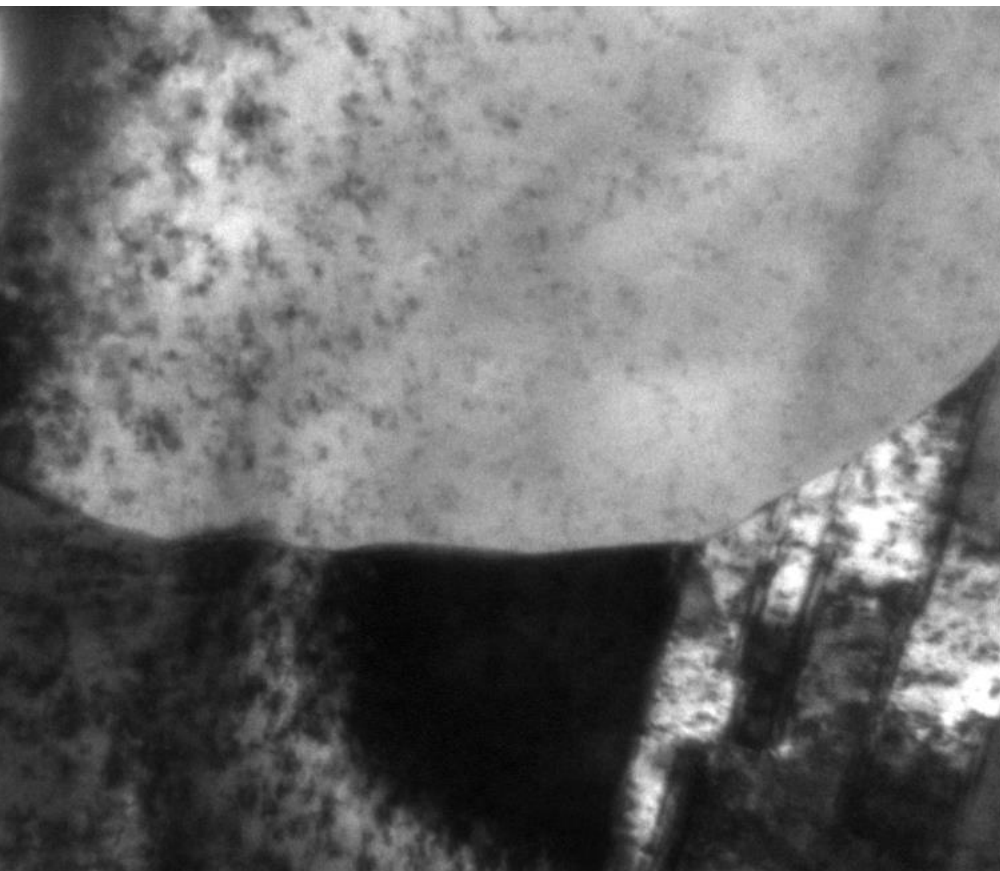
Grain oriented for
channeling

At this tilt, this area
appears to be less
damaged.. I tilted
approximately 1
degree away and
imaged again (see
next slide)

Randomly oriented
grains



Only about one degree tilt from the previous image shows that these areas are actually heavily damaged. This is a nice example of why defect analysis in TEM is challenging and requires very precise imaging conditions.



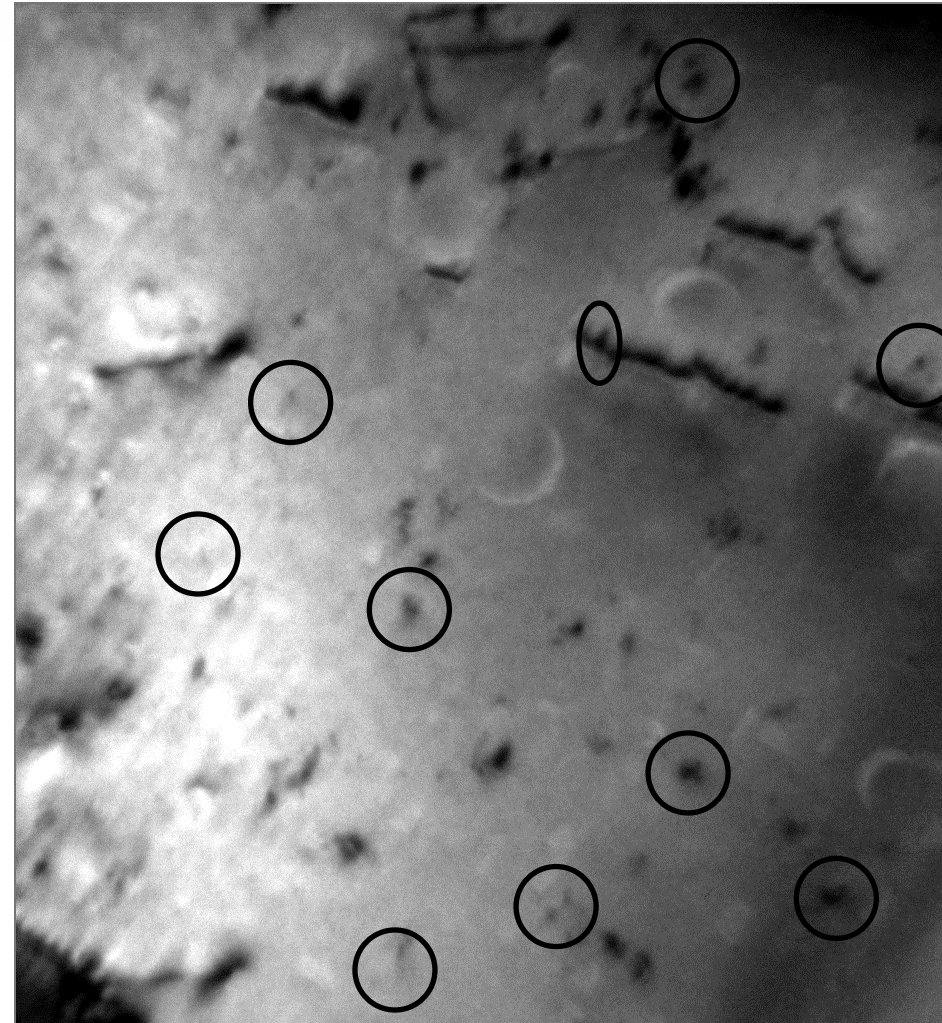
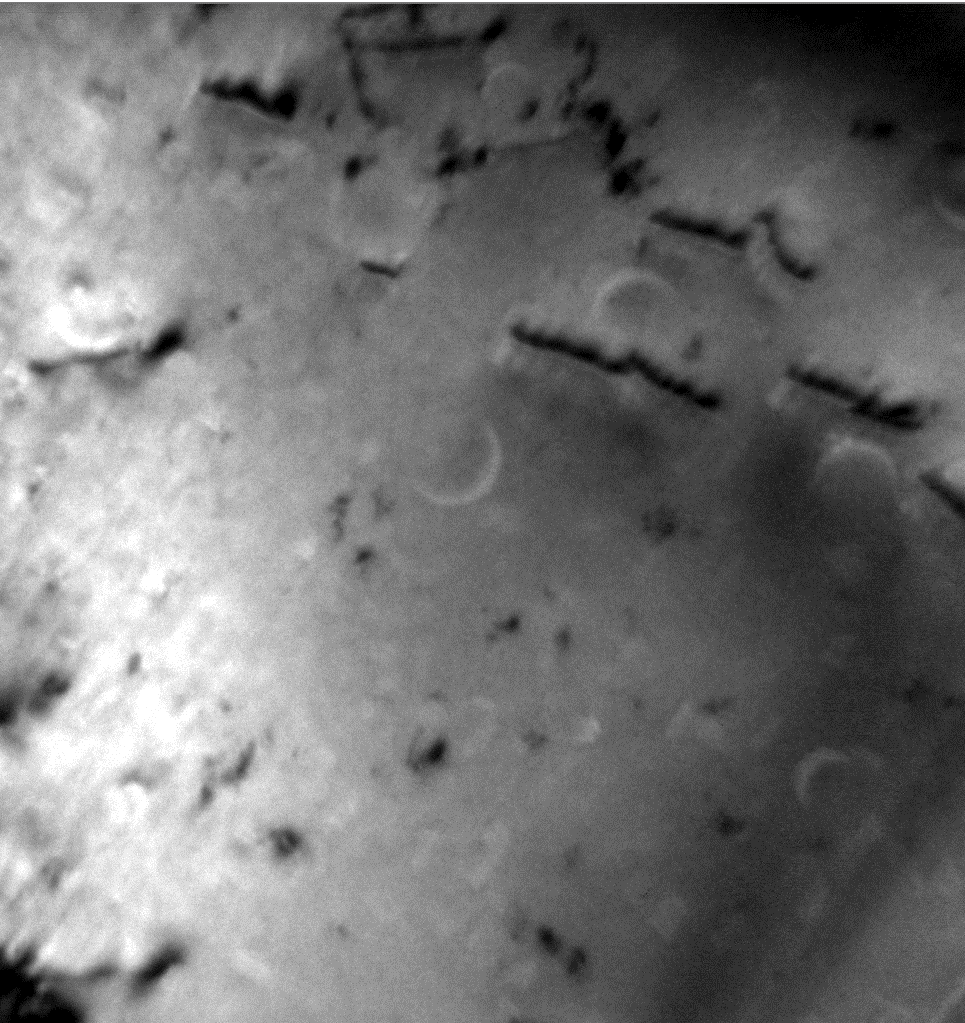
I think these experiments should be run again at a lower current so I can try to actually quantify defect density, but so far I do not see any obvious evidence of channeling...



2.7 MeV Si on Au Channeling Experiment

h	k	l	$\Psi_{1/2}^a$	$\Psi_{1/2}^p$
			axis-deg	plane-deg
0	0	1	2.03	0.43
0	1	1	2.63	0.55
1	1	1	1.35	0.48

2.7 MeV Si on fcc Au 1) $\langle 111 \rangle$ channeled and then 2) random orientation for approximately the same ion fluence. The defects added are circled in the random micrograph, and we expected a lot more?



Why are we not seeing channeling?

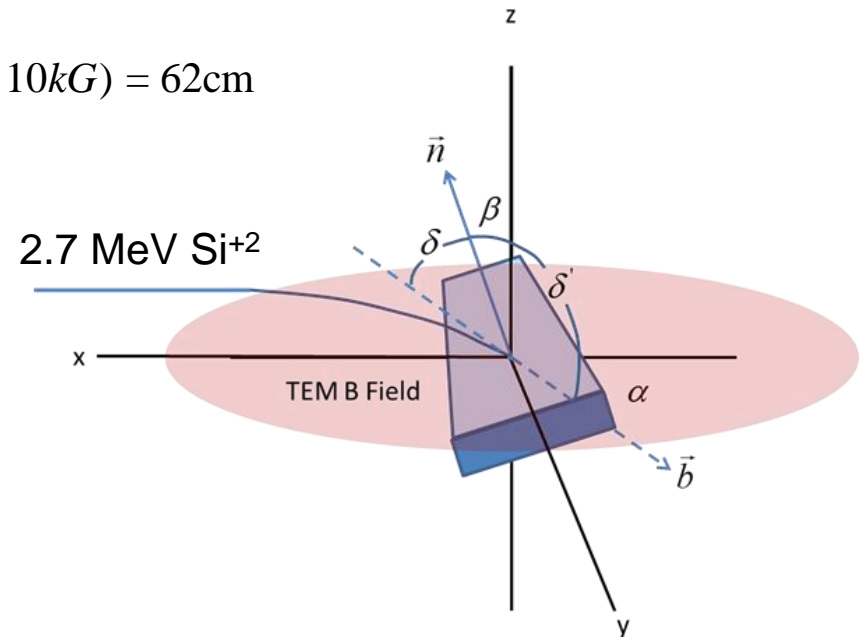
- Sample issues/contamination?
- Could we pick a different axis oriented for channeling which has a larger half angle than the $\langle 111 \rangle$?
- Maybe try a different ion or energy?
- Maybe try a BCC metal so there is a lot more room for error in alignment
- Are we super certain the beam enters perfectly orthogonally to the stage?
- Are we sure the magnetic field in TEM doesn't change affect direction beyond half angle
- Do our tandem ions have energies below the minimum energy for channeling (ala Hobler)

The B field in the TEM can change the angle of the beam ~ the same as the channeling 1/2 angles

$$R_T = \frac{\sqrt{2mE}}{B_T q} = (\text{for } m=28, q=2, E=2.7 \text{ MeV}, B_T = 10 \text{ kG}) = 62 \text{ cm}$$

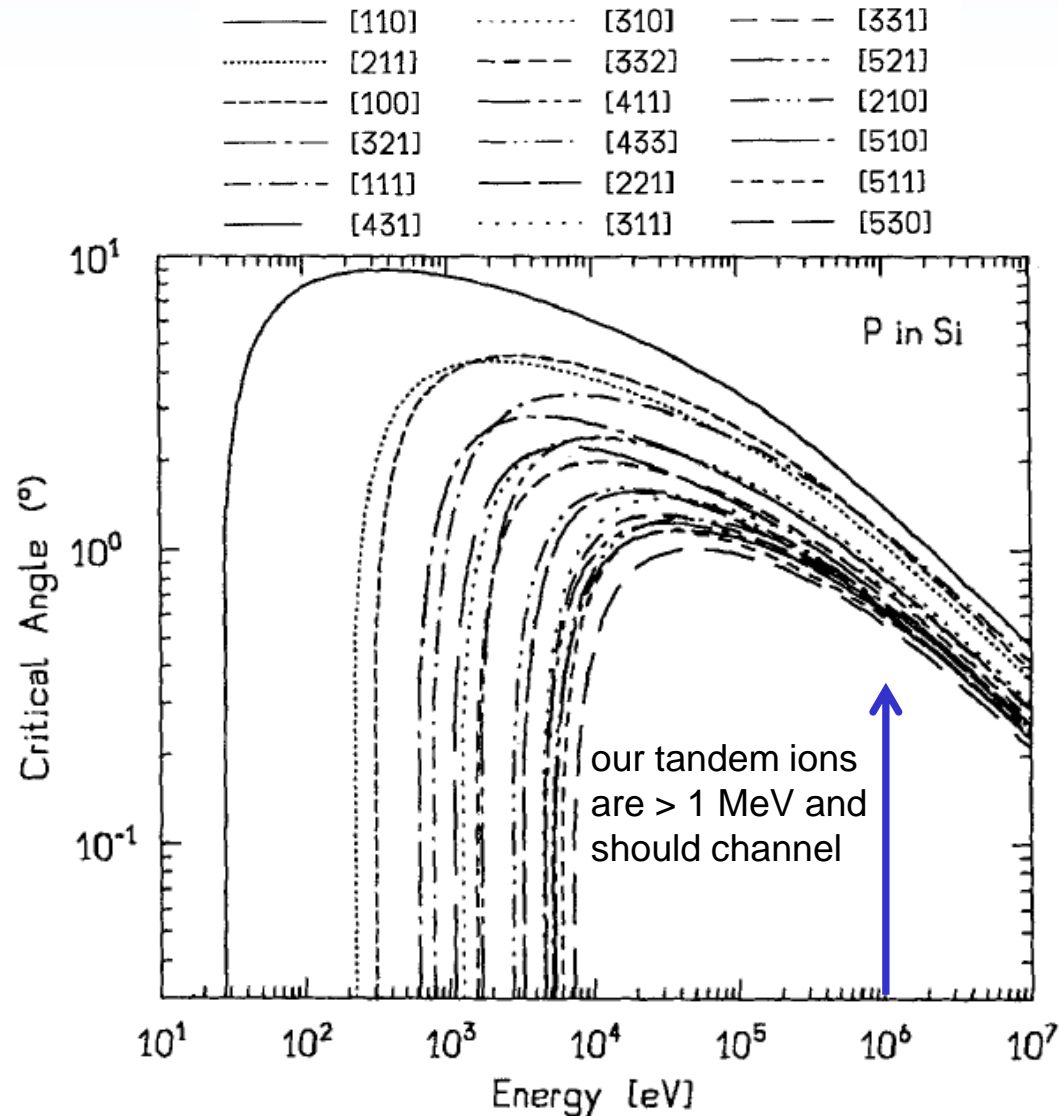
$$r_T = 2 \text{ cm}$$

$$\alpha = \tan^{-1} \left(\frac{dy}{dx} \right) = \tan^{-1} \left(\frac{r_T}{R_T} \sqrt{\frac{1 + \frac{1}{2} \left(\frac{r_T}{R_T} \right)^2}{1 - \frac{1}{2} \left(\frac{r_T}{R_T} \right)^2}} \right) = 1.8^\circ$$



h	k	l	$\Psi_{1/2}^a$ axis-deg	$\Psi_{1/2}^p$ plane-deg
0	0	1	2.03	0.43
0	1	1	2.63	0.55
1	1	1	1.35	0.48

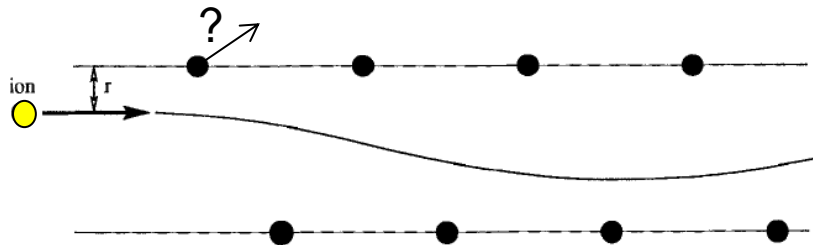
Hobler has calculated lower energy limits to ion channeling



Why are we not seeing channeling? (a more sinister possibility ☹)

- The premise that RBS channeling doesn't displace atoms is wrong?
 - then the $\Psi_{1/2}$ s are wrong
 - => new "nondamaging" channeling theory

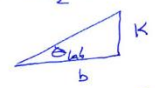
In the standard Lindhard and Hobler channeling theories, the target atoms are replaced by fixed lines of charge. ...But do these atoms really remain fixed during the ion's closest approach?



$$r_{\text{crit}}^0 = 2/3 \cdot a \sqrt{\alpha} (1 - \sqrt{\alpha}/19 + \alpha/700) \text{ with } \alpha = Z_1 Z_2 e^2 d_R / a^2 E$$

Binary collision of 1 MeV Si on Si with an impact parameter b equal to r_{crit}^0

Handwritten calculations in a document viewer window:

$m_1 = m_2$
 Marion (9.57) $b = K \cot(\theta_{\text{cm}})$
 $\therefore \theta_{\text{cm}} = 2 \cot^{-1} \frac{b}{K}$
 (9.96) $\theta_{\text{lab}} = \frac{\theta_{\text{cm}}}{2} = \cot^{-1} \left(\frac{b}{K} \right)$

 $\frac{E_{\text{lab}}}{E_{\text{recoil}}} \approx \frac{K}{b}$
 (9.266) $\frac{T_2'}{T_0 E} = \sin^2(\theta_{\text{lab}})$
 $T_2 = E_{\text{recoil}} \sin^2 \left(\frac{K}{b} \right) \approx E \left(\frac{K}{b} \right)^2$
 (9.49) $K = \frac{K}{2T_0} = \frac{Z_1 Z_2 e^2}{E}$
 (9.16b) $T_2' = \frac{1}{2} T_0 = \frac{1}{2} E$
 for high E say $> 0.1 \text{ MeV}$
 Hobler (34) $b \approx \frac{2}{3} a \alpha^{1/2}$
 $= \frac{2a}{3} \sqrt{\frac{Z_1 Z_2 e^2 d_R}{a^2 E}}$
 $E_{\text{recoil}} \approx E \frac{K^2}{b^2} = \frac{E \left(\frac{Z_1 Z_2 e^2}{E} \right)^2}{\frac{4a^2}{9} \left(\frac{Z_1 Z_2 e^2 d_R}{a^2 E} \right)} = \frac{9 Z_1^2 Z_2^2 e^4}{4 d_R} \approx 1.4 \times 10^{-14} \text{ J}$
 $= 0.0012 \text{ MeV}$

Yikes!



Summary

- Developed Excel program for calculating unintentional ion channeling probability in
 - randomly oriented polycrystalline materials
 - textured materials
 - need beam-sample geometry (including ion steering by TEM)
 - orientation microscopy data ($\varphi_1, \Phi, \varphi_2$)
- ...but may need a new theory for axial and planar $\Psi_{1/2}$ where displaced atoms are not made
- ...and if you are OK with the RBS $\Psi_{1/2}$ s approach, I'll be glad to calculate channeling probabilities for you. bldoyle@sandia.gov