

Introduction to ORDER:

ORientation Definition Extending to Reciprocal space Software for the PEAXIS instrument at Helmholtz Zentrum Berlin

> Version 1.0 by Maciej Bartkowiak

07/06/21

ORDER User Guide - PEAXIS Instrument

Foreword

ORDER software was created as a tool for the users of the PEAXIS instrument at the Helmholtz Zentrum Berlin.

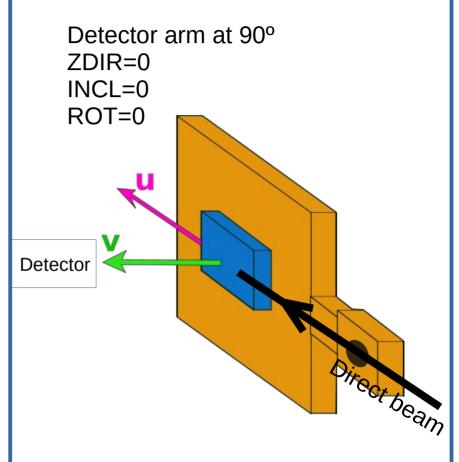
If you want to measure a powder/polycrystalline sample, or you never heard of a "UB matrix" before, then this software will not be of critical importance to you.

ORDER is written in Python and licensed under GNU GPL v3. This means that it is free software, and you are entitled (and encouraged) to download and read the source code of ORDER. If you re-use parts of this code in your own software and release the software to the users, you will have to make the source code available too.

The sample orientation on the PEAXIS instrument is largely preconditioned by the orientation on the sample holder itself.

The **u** and **v** vectors correspond to those defined by Busing and Levy in their paper: Acta Crystallographica **22**, 457 (1967) DOI: 10.1107/S0365110X67000970

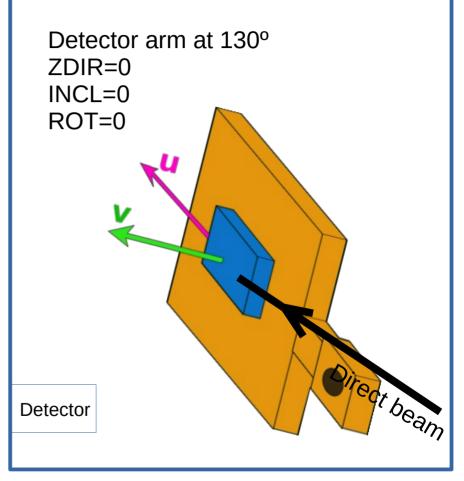
The **u** and **v** used by ORDER are identical to the Busing and Levy definition when the detector arm is at 90 degrees, and the 3 rotation angles of the manipulator are set to 0.



ORDEF

The entire sample chamber, including the manipulator, is tilted around the beam direction when the detector arm moved away from the 90° position. The tilt angle is a function of the detector arm position. If a specific sample orientation has to be maintained, the manipulator motors are used to compensate for the tilting.

The main feature of ORDER is that it can tell the users how to reach a specific position in the reciprocal space, and it compensates for the chamber tilt at the same time.



ORDER

The capabilities of ORDER.

Definition of the sample unit cell and orientation on the holder can be specified here. Critical for single-crystal samples.

The most important tab: it can calculate the motor positions of the instrument needed to create the desired scattering geometry. You can choose which parts of the geometry are fixed, depending on which parameters are important in your experiment.

ORDER: ORientation Definition Extending to Reciprocal space

From motors to HKL Flexible orientation finder Sample Definition

Offsets Total Coverage

This tab can take the instrument parameters and tell you where in the reciprocal space you are.

This tab can be used to correct the sample orientation by offsets based on the specular reflection position.

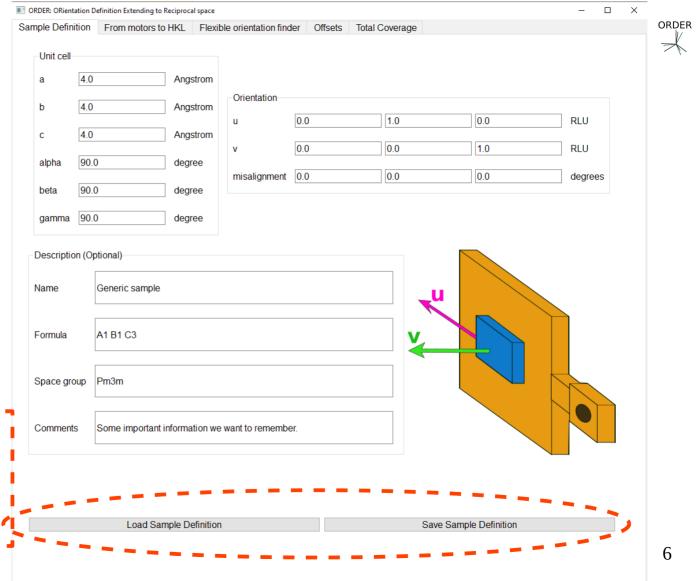
Shows the entire coverage of the instrument. Useful in the early stages of experiment planning, to check if your experiment is feasible.

Sample Definition

As the first step, it is necessary to define the crystallographic unit cell of the sample.

Save your sample definition to a file. You can load it later, or share it with the instrument scientists.

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From motors to HKL

The input here consists of the manipulator motor positions, and the incoming photon energy.

Additionally, the sample definition is copied from the first tab.

The calculated output shows:

1. The current position in the reciprocal space,

2. The absolute value of the Q vector,

3. The angle **theta** between the incoming beam and the sample surface.

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mple Definition	From motors	o HKL Fr	om HKL to motors	Flexible orientat	ion finder	Offsets Tot	al Coverage	
-Sample (read-	only)						., ., ., .	
						1.0	X vs. Y scatteri	
а	4.0		Angstrom			0.5		
b	4.0		Angstrom	Manipulator		0.5		Uideal
				xpos 5.0	mm	0.0	\rightarrow	Q
С	4.0		Angstrom	ypos 5.0	mm			Ureal Vreal
alpha	90.0		degree	ypos <u>3.0</u>		-0.5		
				zpos 5.0	mm	-1.0	0.5 0.0	0 -0.5 -1.0
beta	90.0		degree	zdir 45.0	dograa			
gamma	90.0		degree	zdir 45.0	degree	* ←	→ + Q =	
5				incl 0.0	degree			
u	0.0 1.0	0.0	RLU	rot 0.0	dograa	1.0	Z vs. Y scatteri	
v	0.0 0.0	1.0	RLU	rot 0.0	degree	0.5		
						0.5		Uideal
misalignment	0.0	0.0	degrees			0.0		Q Ureal
						-0.5		
						-0.5		
		-Output-				-1.0	0.5 0.0	0 -0.5 -1.0
Scattering		HKL	-0.0	0.38919	RLU	* ←	→ + Q =	
Ei 85	53.0 eV	dHKL	0.00085 0.00	079 0.00079	RLU		Z vs. X scatteri	ing geometry
						1.0	— -k _i	
Ef_min 84	40.0 eV	Q	0.61133		AA^(-1)	0.5	— k _f	
Ef_max 86	66.0 eV	Q_perp	0.61133		AA^(-1)		Uideal Videal	
arm_theta 90	0.0 degree	Q par	0.0]	AA^(-1)	0.0	Q Ureal	
uni_inclu 50		, <u> </u>	0.0		, v (- i)	-0.5	Vreal	
		theta	45.0		deg.	-1.0		
						1.0	0.5 0.0	0 -0.5 -1.0

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From motors to HKL

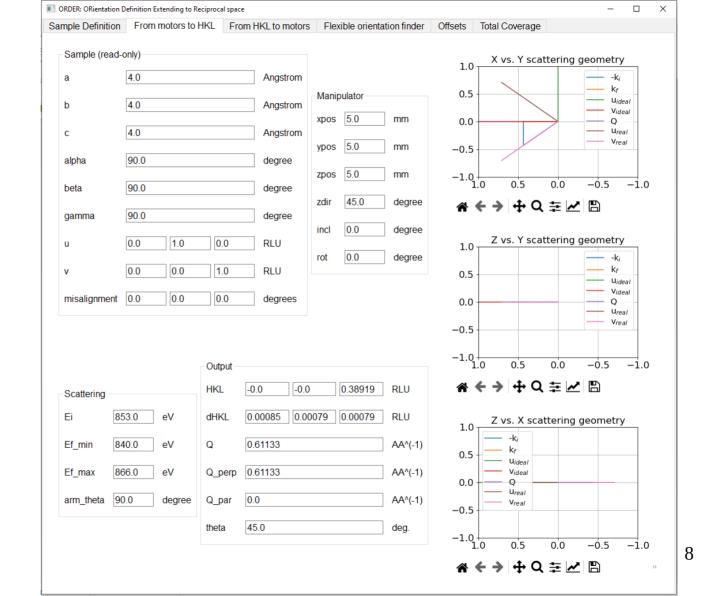
The scattering vector Q is also decomposed into two components, Q_perp and Q_par.

Q_perp is the component of Q that is perpendicular to the sample surface (i.e. the projection of Q onto the normal vector of the sample surface.)

Q_par is the component of Q in the sample surface plane.

 $Q^2 = Q_par^2 + Q_perp^2$

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The FIXED parameters are those that must remain at the specified value. For example, if you want to use the 853 eV photon energy, keep it FIXED at that value.

The software will calculate the manipulator motor positions needed to reach the target.

Only the solutions with CostFunction=0 are correct.

r.	DER: ORientation D	erinition Extending	to Reciprocal space	e				
n	ple Definition	From motors	s to HKL Fro	om HKL	to moto	ors Fle	exible	e orientation find
A	All parameters -							
	5	853.0		eV	<-	FIXED!		Sample (read-
F	4	-0.21778		RLU	□ <- [FIXED!		а
								b
k	<	0.0		RLU	⊻ <- I	FIXED!		
L		0.44878		RLU	□ <- [FIXED!		С
lr	n-plane vector	1.0 0.0	0.0	RLU	⊻ <- [FIXED!		alpha
C	2	0.78355		AA^(-1)		FIXED!		beta
C	Q_par	0.34208		AA^(-1)		FIXED!		gamma
C	2_perp	0.70494		AA^(-1)		FIXED!		u
tł	heta	39.11417		degree	□ <- F	FIXED!		
_	rm thata	(100 a)		degree				V
a	irm_theta	130.0		degree	⊻ <-1			misalignment
	1	2	3	4		5		
1	CostFunction	ArmTheta	ZDIR	INCL		ROT		
2	0.0	130.0	39.491141	-7.2547	788	95.9411		Output (read-or
3	0.0	130.0	85.669971	-0.7135	549	99.34		zdir
1	0.0	130.0	0.345522	-9.3668	317	90.0562		
5	0.0	130.0	43.877763	-6.7808	867	-83.5226		incl
3	0.0	130.0	154.444254	12.144	951	94.0344		rot
7	0.0	130.0	154.659657	8.9060	35	-86.0054		101
3	0.0	130.0	155.039062	3.3046	88	-86.0449		Cost function
9	0.0	130.0	154.003472	1.5427	4	94.0066		

Offsets Total Coverage only) 40 Anastrom 4.0 Angstrom 4.0 Anastrom 90.0 degree 90.0 degree 90.0 dearee 0.0 1.0 0.0 RLU 0.0 0.0 1.0 RLU 0.0 0.0 0.0 degrees

 $\Box \times$

Output (read-o	only)	
zdir	39.49114	degree
incl	-7.25479	degree
rot	95.94115	degree
Cost function	0.0	N/A

Calculate!

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If the FIXED parameters are mutually exclusive, there will be no solution with CostFunction=0. It means that it is not possible to find a sample orientation that will satisfy all the requirements.

It is also possible to have many correct solutions. You can compare them, and pick the best one.

] (ORDER: ORientation D	efinition Extendin	g to Reciprocal spa	ce							- C	
Sa	mple Definition	From motor	rs to HKL Fr	om HKL to mo	tors Fle	exible orientation find	der	Offsets Total (Coverage			
	All parameters											
	Ei	853.0		eV	- FIXED!	Sample (read-	-only)-					
	н	-0.21778		RLU □<	- FIXED!	а	4.0				Angstron	n
	к	0.0		RLU ⊠ <	- FIXED!	b	b 4.0				Angstron	n
	L	0.44878		RLU □<-	- FIXED!	с	4.0				Angstron	n
	In-plane vector	Dr 1.0 0.0 0.0		RLU ⊠ <- FIXE		alpha	90.0				degree	
	Q	0.78355		AA^(-1) □ <- FIXED!		beta	90.0				degree	
	Q_par	0.34208		AA^(-1) □ <- FIXEI		gamma	90.0	90.0			degree	
	Q_perp	0.70494		AA^(-1) □ <- FIXE		u	0.0	0.0 1.0 0.0		.0	RLU	
	theta	heta 39.11417		degree □ <- FIXED!		v	0.0	.0 0.0 1.0		.0	RLU	
	arm_theta	arm_theta 130.0		degree		misalignment	0.0	0.0	0	.0	degrees	
	1	2	3	4	5							
İ	1 CostFunction	ArmTheta	ZDIR	INCL	ROT							
	2 0.0	130.0	39.491141	-7.254788	95.9411	Output (read-o	inly)					
	3 0.0	130.0	85.669971	-0.713549	99.34	zdir	39.49	9114	degree			
	4 0.0	130.0	0.345522	-9.366817	90.0562		7.05					
	5 0.0	130.0	43.877763	-6.780867	-83.5226	incl	-7.25	6479	degree			
	6 0.0	130.0	154.444254	12.144951	94.0344	rot	95.94	4115	degree			
	7 0.0	130.0	154.659657	8.906035	-86.0054				0			
١	8 0.0	130.0	155.039062	3.304688	-86.0449	Cost function	0.0		N/A			
1	0.0	130.0	154.003472	1.54274	94.0066							
								Calcula	atol			
								Calcula	ate!			
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L	<				>]						

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The "in-plane vector" is a reciprocal space vector that should be kept in the scattering plane of the instrument.

By keeping this vector fixed in your experiment, you can have the software compensate for the sample chamber tilt by applying a rotation around the **v** vector. Many users like to keep the **u** vector in the scattering plane.

All parameters Ei 853.0 eV I<	
H 0.21778 RLU C FIXED! a 4.0 K 0.0 RLU C FIXED! b 4.0 L 0.44878 RLU C FIXED! c 4.0 In-plane vector 1.0 0.0 0.0 RLU C FIXED! c 4.0 Q 0.78355 AA^(-1) C FIXED! c 4.0 0.0 Q_perp 0.34208 AA^(-1) C FIXED! alpha 90.0 90.0 Q_perp 0.70994 AA^(-1) C FIXED! gamma 90.0 0.0 1.0 0.0 atria 10.0 39.11417 degree C FIXED! u 0.0 1.0 0.0 1 2 3 4 5 NCL ROT nisalignment 0.0 0.	
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Q_par 0.34208 AA^(-1) □ <- FIXED!	degree
Q_perp 0.70494 AA^(-1) □ <- FIXED!	degree
theta 39.11417 degree <- FIXED!	degree
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arm_theta 1000 degree ⊠ <- FIXED!	
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9 0.0 130.0 154.003472 1.54274 94.0066	
Colviatel	
Calculate!	

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Theta is the angle between the incoming photon beam and the surface of the sample.

Theta=90° is normal incidence.

Theta=0° is (fully) grazing incidence.

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In a real-life experiment a non-zero value of theta is needed to observe signal in the detector.

ampl	le Definition	From motor	s to HKL Fr	om HKL	to motors	; Fle	xible orientation fine	der Offsets	s Total	Covera	ge	
All	parameters											
Ei		853.0		eV	⊠ <- FI)	KED!	Sample (read-	-only)				
н		-0.21778		RLU	□ <- FI)	KED!	а	4.0				Angstro
к		0.0		RLU	⊠ <- FI)	KED!	b	4.0				Angstro
L		0.44878		RLU	□ <- FI)	KED!	с	4.0				Angstro
In-j	plane vector	1.0 0.0	0.0	RLU	⊠ <- FI)	KED!	alpha	90.0				degree
Q		0.78355		AA^(-1)	🗆 <- FI)	KED!	beta	90.0				degree
Q_	_par	0.34208		AA^(-1)	□ <- FI)	KED!	gamma	90.0				degree
Q_	_perp	0.70494		AA^(-1)	□ <- FI)	KED!	u	0.0	1.0		0.0	RLU
the	eta	39.11417		degree	🗆 <- FI)	KED!						_
	m thata			dograa	■		v	0.0	0.0		1.0	RLU
an	m_theta	130.0		degree	≥ <- Fb	NED!	misalignment	0.0	0.0		0.0	degrees
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20		130.0 130.0	39.491141	-7.2547		5.9411				1		
30			85.669971	-0.7135		9.34	zdir	39.49114		degr	ee	
40		130.0	0.345522	-9.3668		0.0562	in al	-7.25479		degr	ee	
50		130.0	43.877763	-6.7808		3.5226						
60		130.0	154.444254	12.144		4.0344	rot	95.94115		degr	ee	
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									Calcul	atel		
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						*						

ORDER: ORientation Definition Extending to Reciprocal space

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Offsets

This tab can only be used once you have experimentally confirmed that the specular reflection is not exactly at the expected positon.

Once you have input some positions at which you found the real specular reflection, you can fit and extrapolate them to other detector arm angles, and predict the offsets needed to find it at those angles.

ORDER: ORientation Definition Extending to Reciprocal space From motors to HKL From HKL to motors Flexible orientation finder Offsets Total Coverage Sample Definition Add from file Save to file Clear table 2 3 Λ ArmTheta ZDIR INCL ROT Usel 0.0 0.0 0.0 \checkmark 2 -10 3 -10 0.0 0.0 0.0 \sim -1.0 0.0 0.0 0.0 \sim -10 0.0 0.0 0.0 \checkmark 5 6 -1.0 0.0 0.0 0.0 \checkmark 7 -1.0 0.0 0.0 0.0 \checkmark **☆ ← →** ⊕ Q ☲ 🖊 🖺 8 -10 0.0 0.0 0.0 \checkmark 0.0 \checkmark 9 -1.0 0.0 0.0 10 -1.0 0.0 0.0 0.0 \checkmark \checkmark 11 -1.0 0.0 0.0 0.0 12 -1.0 0.0 0.0 0.0 \checkmark 13 -1.0 0.0 0.0 0.0 \sim **+ Q ≒ ⋈** 問 Output Input zdir 0.0 degree 90.0 arm theta dearee incl 0.0 degree poly order 0 N/A 0.0 rot degree ╋Q╪╱╚ Plot positions Fit offsets

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Total coverage

This tab calculates all the Q vector values that can be reached by PEAXIS for a specific photon energy. The different Q values are reached by moving the detector arm.

Some important K-edges (blue) and L-edges (red) are included in the plot.

