P. STADELMANN JEMS-SWISS CHEMIN ROUGE 15 CH-1805 JONGNY SWITZERLAND

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### 1. INTRODUCTION

The indexing of SAED patterns can be made faster by the full use of jems functions. In particular, jems contains tools for indexing regular spot and Kikuchi line diffraction patterns. Generally speaking, the indexing consists of determining the  $(\mathbf{h}, \mathbf{k}, \mathbf{l})$  indices of the reflections and calculating the zone axis  $[\mathbf{u}, \mathbf{v}, \mathbf{w}]$  indices. It is always a good idea to put the experimental SAED patterns and the related crystal files in a single folder. The indexing uses the ratios of the length of 2 or 3 SAED vectors, and their angles. Though the exact knowledge of the microscope accelerating voltage and camera length is not necessary to index diffraction patterns, knowing their values accelerates the indexing process, since only a reduced set of (h,k,l) reflections, compatible with these microscope parameters, is generated and scanned to determine the  $(\mathbf{h},\mathbf{k},\mathbf{l})$  reflections that provide the proper ratios and angles. When not specified, the whole set of reflections that the microscope can transmit (limited by the objective lens acceptance angle) is scanned. Such a set of (h,kl,) reflections may contain several hundreds or thousands of reflections. Reducing the acceptance angle of the microscope by specifying the microscope parameters accelerates the indexing process. The  $[\mathbf{u}, \mathbf{v}, \mathbf{w}]$  zone axis indices are calculated using the vector product of the indexed reflections.

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The indexing process can consider several different crystal structures, and provides possible solutions as a stereogram or table for each structure.

## 2. SAED indexing using a table of zone axis patterns

The frame displaying the stereographic projection of GaN (Fig. 1) allows to tabulate the zone axis pattern (ZAP) of the standard stereographic triangle.



FIGURE 1. The stereographic projection of GaN. The **Tabulate** icon (1) creates a table of zone axis patterns.

The ZAP table's entries show the ratio and angle of the 2 shortest reflections  $(g_1$  and  $g_2)$  of the ZAP as well as their structure factor (amplitude) and the radius of several High Order Laue Zones (HOLZ) (Fig. 2). When the structure factor of either  $g_1$  or  $g_2$  is null the ratio of the next reflections is provided.

Lone and geometry									1		
[u,v,w]::[u,v,t,w]	g1::(h,k,l)	Vg1 Volt	g1   nm-1	q2::(h,k,l)	Vg2 Volt	g2   nm-1	g1 / g2	g2 / g1	<(q1, q2)	FOLZ nm-1	50
[1, 0, 0]::[2, -1, -1, 0]	(0, 1, 0)	8,978	3.621	(0, 0, -1)	0.000	1.929	1.88:: 0.94	0.53:: 1.07	90,000	56.702	80.
[0, 0, 1]::[0, 0, 0, 1]	(0, -1, 0)	8,978	3,621	(-1, 0, 0)	8,978	3.621	1,00	1,00	60,000	44,388	62.
[2, 1, 0]::[1, 0, -1, 0]	(1, -2, 0)	10,723	6.272	(0, 0, 2)	13,396	3.857	1.6.3	0.62	90,000	42.999	60.
[1, 0, 1]::[2, -1, -1, 3]	(0, 1, 0)	8,978	3.621	(1, 0, -1)	7,781	4.102	0.88	1.13	63,813	40.950	58.
[2, 1, 1]::[1, 0, -1, 1]	(-1, 1, 1)	7.604	4.102	(0, 1, -1)	7,781	4.102	1.00	1.00	80,300	36.689	51.9
[2, 0, 1]::[4, -2, -2, 3]	(0, 1, 0)	8,978	3.621	(1, 0, -2)	4.954	5.291	0.68	1.46	69.989	35,218	49.1
[3, 1, 0]::[5, -1, -4, 0]	(1, -3, 0)	3.105	9.580	(0, 0, 1)	0.000	1.929	4.97:: 2,48	0.20:: 0,40	90,000	34.759	49.
[3, 1, 1]::[5, -1, -4, 3]	(1, -1, -2)	4.954	5,291	(0, -1, 1)	7,604	4.102	1.29	0.78	92,334	32.075	45.
[1, 0, 2]::[2, -1, -1, 6]	(0, -1, 0)	8,978	3.621	(-2, 1, 1)	0,000	6.561	0.55:: 0.28	1.81:: 3.62	90,000	30,641	43.
[3, 0, 1]::[2, -1, -1, 1]	(0, 1, 0)	8,978	3.621	(1, 0, -3)	7,880	6.826	0.53	1.89	74,618	30.595	43.
[4, 1, 0]::[7, -2, -5, 0]	(1, -4, 0)	1.849	13.055	(0, 0, 1)	0.000	1.929	6.77:: 3,38	0,15:: 0,30	90,000	29.761	42.
[2, 1, 2]::[1, 0, -1, 2]	(1, -2, 0)	10,723	6.272	(-1, 0, 1)	7,604	4,102	1.53	0.65	90,000	29.441	41,6
[4, 2, 1]::[2, 0, -2, 1]	(0, 1, -2)	4.954	5.291	(1, -1, -2)	4.954	5.291	1.00	1.00	72,700	28.886	40.
[4, 1, 1]::[7, -2, -5, 3]	(0, 1, -1)	7,781	4.102	(1, -1, -3)	7,880	6.826	0.60	1.66	80.537	28,412	40.
[3, 1, 2]::[5, -1, -4, 6]	(1, 1, -2)	6.885	7.363	(1, -1, -1)	7,781	4.102	1.79	0.56	75,742	27.596	39.
[4, 0, 1]::[8, -4, -4, 3]	(0, 1, 0)	8,978	3.621	(1, 0, -4)	1,757	8,522	0.42	2,35	77,734	27,190	38.
[5, 2, 0]::[8, -1, -7, 0]	(2, -5, 0)	1.253	15.783	(0, 0, 1)	0,000	1.929	8.18:: 4.09	0.12:: 0,24	90.000	27.061	38.
[3, 0, 2]::[2, -1, -1, 2]	(0, -1, 0)	8,978	3.621	(-2, 1, 3)	0.000	8,533	0.42:: 0,21	2.36:: 4,71	90,000	26.860	38.
[5, 1, 0]::[3, -1, -2, 0]	(1, -5, 0)	2,240	16.593	(0, 0, 2)	13,396	3.857	4.30	0.23	90,000	26.391	37.
[5, 2, 1]::[8, -1, -7, 3]	(0, -1, 2)	5.035	5,291	(-1, 2, 1)	0,000	6.561	0.81:: 0.40	1.24:: 2.48	110.624	26.193	37.
[4, 1, 2]::[7, -2, -5, 6]	(-1, 0, 2)	5.035	5.291	(-1, 2, 1)	0.000	6.561	0.81:: 0.40	1.24:: 2.48	77.625	25.638	36.
[5, 1, 1]::[3, -1, -2, 1]	(1, -1, -4)	1.757	8,522	(0, -1, 1)	7,604	4.102	2.08	0.48	103,772	25.619	36.
[1, 0, 3]::[2, -1, -1, 9]	(0, 1, 0)	8.978	3.621	(3, -1, -1)	3,172	9.772	0.37	2,70	79.323	25.317	35.
[2, 1, 3]::[1, 0, -1, 3]	(-3, 0, 2)	3,771	11.527	(-1, 2, 0)	10,723	6,272	1.84	0.54	90,000	24.829	35.
[5, 0, 1]::[10, -5, -5, 3]	(0, 1, 0)	8.978	3.621	(1, 0, -5)	4.582	10,301	0.35	2.84	79.877	24.636	34,
[2, 0, 3]::[4, -2, -2, 9]	(0, 1, 0)	8,978	3.621	(3, -1, -2)	2.209	10.327	0.35	2.85	79.904	24.603	34.
[5, 2, 2]::[8, -1, -7, 6]	(-2, 2, 3)	5.268	9.269	(0, 1, -1)	7.781	4.102	2.26	0.44	87.058	24.223	34.
[6, 3, 1]::[3, 0, -3, 1]	(-1, 2, 0)	10,723	6.272	(0, 1, -3)	7,880	6.826	0.92	1.09	62.650	24.208	34.
[6, 2, 1]::[10, -2, -8, 3]	(-1, 2, 2)	6.993	7.363	(0, 1, -2)	4.954	5.291	1.39	0.72	82.940	24.008	33.
[3, 1, 3]::[5, -1, -4, 9]	(1, -3, 0)	3.105	9.580	(-1, 0, 1)	7.604	4.102	2,34	0.43	80,398	23.979	33.
[6, 1, 0]::[11, -4, -7, 0]	(1, -6, 0)	0.690	20.160	(0, 0, 1)	0.000	1.929	10.45:: 5.23	0.10:: 0.19	90,000	23.939	33.
[5, 1, 2]::[3, -1, -2, 2]	(0, -2, 1)	4.202	7,494	(-1, 1, 2)	5.035	5.291	1.42	0.71	98.224	23.829	33.
[6, 1, 1]::[11, -4, -7, 3]	(-1, 2, 4)	3.009	9.942	(0, 1, -1)	7.781	4.102	2.42	0.41	83.259	23.453	33.
[5, 0, 2]::[10, -5, -5, 6]	(0, -1, 0)	8.978	3.621	(-2, 1, 5)	0.000	11.503	0.31:: 0.16	3.18:: 6.35	90,000	23.128	32.
[4, 2, 3]::[2, 0, -2, 3]	(1, -2, 0)	10.723	6.272	(-1, -1, 2)	6.993	7.363	0.85	1.17	64.793	23.092	32.0
[4, 1, 3]::[7, -2, -5, 9]	(1, 2, -2)	2,209	10.327	(1, -1, -1)	7,781	4.102	2.52	0.40	88,805	22.934	32.
17 3 01::[11 -1 -10 0]	(3 -7 0)	0.538	22 0 25	(0 0 1)	0.000	1929	11 42:: 5 71	0.09:: 0.18	90.000	22 901	32.
1											•

FIGURE 2. Zone axis patterns of the standard stereographic triangle: ZAP [uvw] (or [uvtw] hexagonal) indices,  $g_1$  (hkl) indices, its structure factor ([Volt]) and length ( $[nm^{-1}]$ ),  $g_2$  (hkl) indices, its structure factor ([Volt]) and length ( $[nm^{-1}]$ ), their ratio  $g_1/g_2$  and  $g_2/g_1$  and the angle between  $g_1$  and  $g_2$  (< ( $g_1, g_2$ )) and the radius of the first three HOLZ.

A search of ZAPs of similar  $g_1$ ,  $g_2$  ratio and angle is activated by the search tool button<sup>1</sup> (Fig. 3).

S 🖪 📑 👟		9	1 / g2 ratio	0.42							
		(	(g1, g2) angl	e [deg.] <mark>78</mark>							
Zone axis geometry				~ ~ 1				7			
[u,v,w]::[u,v,t,w]	q1::(h,k,l)	Vg1 Volt			Search	2		g2 / g1	<(q1, q2)	FOLZ nm-1	50
[1, 0, 0]::[2, -1, -1, 0]	(0, 1, 0)	8.978			Jearch	<u> </u>		0.53:: 1.07	90,000	56.702	80.
[0, 0, 1]::[0, 0, 0, 1]	(0, -1, 0)	8,978		5-1-1-2				1.00	60,000	44.388	62.
[2, 1, 0]::[1, 0, -1, 0]	(1, -2, 0)	10,723	6.272	(0, 0, 2)	13.396	3.857	1.63	0.62	90,000	42.999	60.
[1, 0, 1]::[2, -1, -1, 3]	(0, 1, 0)	8,978	3.621	(1, 0, -1)	7.781	4.102	0.88	1.13	63,813	40.950	58.
[2, 1, 1]::[1, 0, -1, 1]	(-1, 1, 1)	7.604	4,102	(0, 1, -1)	7.781	4,102	1.00	1.00	80,300	36.689	51.5
[2, 0, 1]::[4, -2, -2, 3]	(0, 1, 0)	8,978	3,621	(1, 0, -2)	4.954	5.291	0.68	1.46	69.989	35.218	49.
[3, 1, 0]::[5, -1, -4, 0]	(1, -3, 0)	3.105	9.580	(0, 0, 1)	0.000	1.929	4.97:: 2.48	0.20:: 0,40	90,000	34.759	49.
[3, 1, 1]::[5, -1, -4, 3]	(1, -1, -2)	4.954	5,291	(0, -1, 1)	7,604	4.102	1.29	0.78	92,334	32.075	45.4
[1, 0, 2]::[2, -1, -1, 6]	(0, -1, 0)	8.978	3.621	(-2, 1, 1)	0.000	6.561	0.55:: 0.28	1.81:: 3.62	90,000	30.641	43.
[3, 0, 1]::[2, -1, -1, 1]	(0, 1, 0)	8,978	3,621	(1, 0, -3)	7,880	6.826	0.53	1.89	74,618	30.595	43.
[4, 1, 0]::[7, -2, -5, 0]	(1, -4, 0)	1.849	13.055	(0, 0, 1)	0.000	1.929	6.77:: 3.38	0.15:: 0.30	90,000	29.761	42.
[2, 1, 2]::[1, 0, -1, 2]	(1, -2, 0)	10,723	6.272	(-1, 0, 1)	7,604	4.102	1.53	0.65	90,000	29.441	41.0
[4, 2, 1]::[2, 0, -2, 1]	(0, 1, -2)	4.954	5.291	(1, -1, -2)	4.954	5.291	1.00	1.00	72,700	28.886	40.
[4, 1, 1]::[7, -2, -5, 3]	(0, 1, -1)	7.781	4.102	(1, -1, -3)	7.880	6.826	0.60	1,66	80.537	28,412	40.
[3, 1, 2]::[5, -1, -4, 6]	(1, 1, -2)	6.885	7,363	(1, -1, -1)	7,781	4.102	1.79	0.56	75,742	27,596	39.0
(4, 0, 11::[8, -4, -4, 3]	(0, 1, 0)	8.978	3,621	(1, 0, -4)	1,757	8.522	0.42	2.35	77.734	27.190	38
[5, 2, 0]::[8, -1, -7, 0]	(2, -5, 0)	1.253	15,783	(0, 0, 1)	0.000	1.929	8.18:: 4.09	0.12:: 0.24	90,000	27,061	38.
[3, 0, 2]::[2, -1, -1, 2]	(0, -1, 0)	8,978	3,621	(-2, 1, 3)	0.000	8,533	0,42:: 0,21	2.36:: 4,71	90,000	26.860	38.
[5, 1, 0]::[3, -1, -2, 0]	(15. 0)	2.240	16.593	(0, 0, 2)	13.396	3.857	4.30	0.23	90.000	26.391	37.
[5, 2, 1]::[8, -1, -7, 3]	(0, -1, 2)	5.035	5.291	(-1, 2, 1)	0.000	6.561	0.81:: 0.40	1.24:: 2.48	110.624	26.193	374
[4, 1, 2]::[7, -2, -5, 6]	(-1, 0, 2)	5.035	5.291	(-1, 2, 1)	0.000	6.561	0.81:: 0.40	1.24:: 2.48	77.625	25.638	36.
[5 1 1]::[3 -1 -2 1]	(114)	1.757	8.522	(0, -1, 1)	7.604	4.102	2.08	0.48	103,772	25.619	36.
[1.0.3]::[211.9]	(0,1,0)	8.978	3.621	(3, -1, -1)	3.172	9,772	0.37	2.70	79.323	25.317	35.
[2 1 3]::[1 0 -1 3]	(-3.0.2)	3.771	11.527	(-1, 2, 0)	10.723	6.272	1.84	0.54	90.000	24.829	35.
(5. 0. 11::[1055. 3]	(0,1,0)	8.978	3.621	(1.05)	4.582	10.301	0.35	2.84	79.877	24.636	34.
[2 0 3]::[4 -2 -2 9]	(0,1,0)	8 978	3.621	(3 -1 -2)	2 209	10.327	0.35	2.85	79 904	24 603	341
[5 2 2]::[8 -1 -7 6]	(-2, 2, 3)	5268	9269	(0, 1, -1)	7 781	4102	2.26	0.44	87.058	24223	34
[6 3 1]::[3 0 -3 1]	(-1, 2, 0)	10.723	6272	(0, 1, -3)	7.880	6.826	0.92	1.09	62 650	24208	34
16 2 11::[10 -2 -8 3]	(-1, 2, 2)	6 993	7363	(0, 1, -2)	4 954	5 2 9 1	1.39	0.72	82 940	24 008	331
(3 1 31/16 JL A 01	(1.3.0)	3105	9.580	(10.0	7.604	4102	2.34	0.43	80 398	23.979	1.11
16 1 01::111 -4 -7 01	(1 -6 0)	0.690	20160	(0, 0, 1)	0.000	1929	10.45:: 5.23	0.10:: 0.19	90,000	23.939	33.
(5 1 2):(3 -1 -2 2)	(0 -2 1)	4 202	7 494	(-1, 1, 2)	5.035	5,291	1.42	0.71	98 224	23.829	33
[6 1 1]::[11 -4 -7 3]	(-1, 2, 4)	3 009	9942	(0, 1, -1)	7 781	4102	2.42	0.41	83 259	23 453	33
(5 0 21::(10 -5 -5 6)	(0 -1 0)	8 978	3.621	(-2 1 5)	0.000	11 503	0.31:: 0.16	318::635	90,000	23128	321
[4 2 3]::[2 0 -2 3]	(1 -2 0)	10.723	6.272	(-1 -1 2)	6 993	7 363	0.85	117	64 793	23.092	32
[4 1 3]::[7 .2 .5 9]	(1, 2, -2)	2 209	10 327	(1 -1 -1)	7 781	4102	2.52	0.40	88.805	22.934	32
[7 3 0]-[11 -1 -10 0]	(3 -7 0)	0.538	22 025	(0, 0, 1)	0.000	1 929	11.42. 5.71	0.09.019	90,000	22 901	32
	ita se ul				. WIRDE		. II stored		- DUIDAL		

FIGURE 3. Using the  $g_1$ ,  $g_2$  ratio  $(g_1/g_2)$  and angle  $(\langle g_1, g_2\rangle)$  ZAPs with similar geometry are selected.

The similar ZAPs are shown with a mouse click on the ZAP line (Fig. 4 and Fig. 5).

<sup>&</sup>lt;sup>1</sup>A ratio specified by a series of real numbers means that one or several reflections proportional to either  $g_1$  or  $g_2$  are kinematically forbidden (this happens for example when a screw axis is perpendicular to the ZAP [uvw] direction).



FIGURE 4. Selection of the [311] ZAP.

FIGURE 5. GaN [311] ZAP.

### 3. Starting the SAED pattern indexing

The following notes assume that the crystal structures have been fully described, i.e. at least lattice parameters, the position of the atoms and, optionally, the space-group or the regular point system code (RPS code). In this example, the indexing folder contains the GaN crystal structure and a GaN SAED pattern to index. The first two steps consist in loading the GaN structure and opening the indexing box, as shown in Fig. 6 and 7. Note also that the indexing can be performed using several jems crystal files (i.e. .txt files only).

jems offers several ways to load SAED patterns. The first one (Fig. 8) consists of loading the image "As is", keeping a one-to-one correspondence between the pixels of the file and the pixels of the displayed pattern. The other 2 possibilities allow the display of a pattern of reduced dimension, obtained either:

- (1) by bilinear interpolation (Interpolation) of the original image.
- (2) or by subsampling (**Subsample**) of the original image (usual binning of the CCD cameras). Subsampling is always a power of 2.

The interpolation method adapts the image size to the display area, while the subsample method adapts the display area to the subsampled image.



FIGURE 6. Loading the GaN crystal structure.

The next step consists of loading and displaying the SAED pattern. Figure 9 shows the dialogue for loading SAED patterns. Several types of images can be loaded (including Gatan Digital Micrograph .dm3 images). Once loaded the pattern is displayed in the indexing window, along with a scale marker that allows scaling of the pattern, and 2 arrows (red and green) that will later point to the reflections used to index it (Fig. 10).

The various controls of the indexing window are organized in several tabs, where the:

- Align tab allows rotating (rotation alignment) of the pointing arrows<sup>2</sup>.
- **Crystals** tab displays a table of crystal files that provide the crystal parameters necessary for the indexing procedure<sup>3</sup>.

 $<sup>^{2}</sup>$ The geometry of the pointing arrows can be changed using the stereogram of the *Mask tab*  $^{3}$ One or more crystals can be selected for the indexing process. They are displayed in alphabetical order.



FIGURE 7. The spot indexing box. The scale marker and the red and green arrows are moved under mouse control.

- Mask tab contains a slider, for changing the mask size, and a stereogram for selecting the pointing arrows geometry<sup>4</sup>.
- Microscope tab allows specification of the accelerating voltage, the camera length and the measurement errors (length and angle)<sup>5</sup>.
- **Options** tab contains the check boxes of the indexing procedure options, and also provides a list of the (x, y) coordinates of the experimental SAED spots when the experimental pattern is processed using the **Find peak** kernel of the **Processing** tab.
- **Processing** tab contains image processing options and features to improve (hopefully) the visibility of spots/lines of the experimental diffraction pattern. A useful one is **Colorize**.
- Scale tab contains controls to calibrate the SAED pattern, and radio buttons to fix several microscope parameters<sup>6</sup>.

 $<sup>^{4}</sup>$ The mask is useful for sorting reflections of SAED patterns involving several phases.

 $<sup>^5\</sup>mathrm{The}$  smaller the errors, the more selective the indexing procedure.

 $<sup>^{6}\</sup>mathrm{Many}$  microscope parameters are automatically set to default vales when a crystal structure is loaded.

Atom	Color Contour Debug Display Font Imaging Indexing Mail Measuring Microscope Miscellary
	Tmage stripe / montage
	Lowest beam amplitude considered for imaging 10-8 0 10-7 10-6 10-5 10-4 10-3 10-2
	Maximum dimension of GUI panels       Maximum dimension of reduced images         400       512       640       •       768       1024         256       512       768       1024
	Maximum image dimension 128 256 384 512 640 768 896 1024 2048 4096
	Maximum map dimension 128 256 384 512 640 768 896 1024 2048 4096
	Pixel size of high resolution images / nm           0.0005         0.001         0.002         0.01         0.02<
	Resize loaded images O As is O Interpolate O Subsample
	Power spectrum       Power spectrum log scale       Inear scale       O       Logarithm scale         O         O         Inear scale
	Java 3D. ✓ Enable Check atom site occupancy □ Enable □ Enable
Save these	preferences ?

FIGURE 8. The **Imaging** preferences panel where the **As is**, **Interpolate** or **Subsample** image loading options can be selected. The dialog is available in menu **Parameters** as menu item **Preferences**.

• **Spots** tab allows changing of the arrows sizes and angles.

When the microscope accelerating voltage and camera length are known, it is best to set these **Microscope** parameters immediately (Fig. 11). Using the mouse the scale marker is moved on to some known calibrated feature; the pointing arrows and their center are set to selected spots. When the selected spot is not closest to the origin, the order of the spot must be specified (**Spot order**).

⊖ O Diffrac	tion file
Experimental	<b>÷</b>
Name 🔺	Date Modified
Al.txt	Thursday, April 17, 2008 6:05 PM
💆 Au_powderPattern.jpg	Sunday, January 22, 2006 7:26 PM
💆 Au_powderPatternSmall.jpg	Sunday, January 22, 2006 7:26 PM
DM_AI_300_2000.txt	Friday, January 18, 2008 5:13 PM
DM_GaNP603DiffCond.txt	Friday, January 18, 2008 4:04 PM
🗐 GaN.txt	Monday, May 17, 2010 3:10 PM
🗐 GaN_sup.txt	Wednesday, January 30, 2008 11:52 AM
🗹 GaNDiffExp.gif	Friday, July 1, 2005 8:48 AM
🗮 KP_Al_300_2000.jpg	Friday, January 18, 2008 4:59 PM
LACBEDSi_113.png	Friday, November 16, 2007 9:31 AM
🛃 Si_31k.tif	Friday, July 1, 2005 8:48 AM
🗮 TiO2RingPattern.jpg	Friday, July 1, 2005 8:48 AM
File Format: Diffract	ion file (.dat, .pn 🛟
	Cancel Choose

FIGURE 9. Selection of the SAED pattern.

After setting the microscope parameters and scaling the SAED pattern, one has to select the crystal structures for indexing <sup>7</sup> (Fig. 12). The buttons at the bottom of the crystal structures table allow inclusion of just one crystal structure for the indexing, all the crystal structures of a folder, suppression one or all except the first in the table.

The indexing process is started by a mouse click on the flash lamp tool (search).

Indexing the SAED pattern using three reflections can help eliminate spurious solutions, even though the third reflection is a linear combination of the first two. The option **Three spots indexing** of the options pane (Fig. 12) puts a third arrow (blue arrow) on the SAED pattern. Use the mouse to point it to a reflection, and set the spot order appropriately (**Spots** pane). When the third selected reflection is not the simple summation of the first (red arrow) and second (green

<sup>&</sup>lt;sup>7</sup>Only jems crystal files (.txt files) can be searched for indexing solutions. When searching .cif files save these files in .txt format after checking their RPS code or space-group.



FIGURE 10. The SAED pattern as loaded in the indexing window.

arrow) reflections, set the **indexing likelihood** to a lower value. When the indexing likelihood is lowered the search will consider a large range of ZAPs.

The **Processing** pane is used to apply various image processing procedures on the SAED pattern. A useful one consists in finding the spots' positions automatically. This is achieved (with the displayed GaN SAED pattern) in the following way:

- (1) Select the **Option** tab of the image processing pane (Fig. 13) and check the **Inverse** check box. The contrast of the SAED pattern will be inversed (maximum of intensity at the reflections' positions).
- (2) Select the **Process** tab of the image processing pane (Fig. 14) and the **FindPeak** image processing process.
- (3) Mouse click on the **Hammer** tool button.

The SAED maxima are located and tabulated in the **Options** pane table (Fig. 15). The indexing option **Snap to maxima** automatically snaps the pattern origin or the arrows at the location of the closest maximum. The **Show mask** option plots circles on the lattice defined by the red and green arrows (Fig. 16). The circles' size is changed using the slider of the **Mask** pane.



FIGURE 11. The microscope parameters of the SAED pattern are specified, as well as the measurement errors and the scale of the SAED pattern.

				Options	🔲 Back	ground	🗹 Sho	w mask	Sn:	up to maxin	na
Crystals			1								
Crystal name	Selected	Crystal filename		Indexing o	ptions						
Al		/jemsMacOSX/jemsMac/jemsData/Experimental/Al.tx		Exte	ended search	h 📒	First qu		ution 📃	Three spo	ts indexing
GaN		/jemsMacOSX/jemsMac/jemsData/Experimental/GaN.									
				Indexing li	ikelihood						-
				0.2	0,4	0.5	0.6	0.7	0,8	0.9	• 1.0
				Deals and it							
				Peak positi	#	×		Y	0	unt	
						-		,	0.		-
	_	) + +									
				Peaks cont	rols						
								A		+	
						256		Ψ	-		

FIGURE 12. Selecting the crystal structures and the indexing options.

# 4. Analyzing the indexing solutions

The possible solutions are shown on stereograms during the indexing process. The indexing is performed by concurrent threads, as shown on Fig. 17. The indexing can be stopped at any time. At the end of the indexing procedure, the solutions are provided on a stereogram or tabulated by pushing the table tool button of the sterogram box (Fig. 18).

When the microscope parameters associated to the SAED pattern are known with good accuracy, the indexing process is much faster and only a reduced set of possible solutions is obtained (Fig. 19).

Selecting an indexing solution (either on the stereographic projection or on the table) allows its comparison to the experimental SAED pattern (Fig. 20). The proposed solution is plotted as a standard jems SAED pattern. The **Rotation** alignment control allows rotation of the calculated pattern (a rotation is calculated but, depending on the reflections pointed by the arrows, a supplementary rotation may be necessary). A comparison with a dynamical calculation can be



FIGURE 13. SAED contrast is inverted.



FIGURE 14. The selection of the **FindPeak** image processing.

immediately performed (select the **Crystal/Matrix** tab of the diffraction window). The **Options** tab of this window are also be used to plot Kikuchi or HOLZ lines, etc.



FIGURE 15. The peaks position are tabulated and can be labelled with the buttons at the botton of the table.



FIGURE 16. Circles are centered on the lattice defined by the red and green arrows.

# 5. Remarks

• Since setting the indexing parameters (i.e. specifying the microscope parameters, calibrating the SAED pattern, moving the arrows, etc) needs to



FIGURE 17. The indexing is performed in concurrent threads.

be performed before starting the indexing process, it is a good idea to save these parameters (i.e. position of the center and of the arrows, etc) using the **Dead mouse** dialog, as shown in Fig. 21. This allows a very fast *replay* of the indexing procedure during a subsequent jems session.

• The indexing of Kikuchi line patterns follows the same scheme, except that 3 Kikuchi pairs are always necessary. The indexing of Kikuchi patterns provides the [**u**,**v**,**w**] indices of the **beam direction** (information necessary to perform the simulation of bright/dark field images of crystalline defects).



			Enlution	with Cabl			
			Solutions	with Gain			
indexing ZA::[u.v.w]	a1::(h.k.l)	a2::(h.k.l)	BD::[u.v.w]	LC::(h.k.l)	Camera length / mm	Likelihood	D
[-1,1,0]	(0, 0, 2)	(1, 1, 0)		- (11)	651.7	1.000	1
[1,-1,0]	(0, 0, 2)	(1, 1, 0)			651.7	1.000	d.
[2,1,0]	(0, 0, 2)	(1, -2, 0)			651.7	1.000	1
[-2,-1,0]	(0, 0, 2)	(1, -2, 0)			651.7	1,000	
[-1,-2,0]	(0, 0, 2)	(-2, 1, 0)			651.7	1,000	1
[1,2,0]	(0, 0, 2)	(-2, 1, 0)			651.7	1,000	
[-7,-5,-1]	(-1, 1, 2)	(-1, 2, -3)			475.2	0.805	Т
[-5,-7,1]	(-1, 1, 2)	(-2, 1, -3)			475.2	0.805	
[5,7,1]	(1, -1, 2)	(2, -1, -3)			475.2	0.805	Т
[7,5,-1]	(1, -1, 2)	(1, -2, -3)			475.2	0.805	
[-2,-7,-1]	(-1, 0, 2)	(-2, 1, -3)			475.2	0.805	Т
[7,2,1]	(0, -1, 2)	(1, -2, -3)			475.2	0.805	ľ
[-7,-2,1]	(0, 1, 2)	(-1, 2, -3)			475.2	0.805	Т
[2,7,-1]	(1, 0, 2)	(2, -1, -3)			475.2	0.805	
[2,-5,1]	(-1, 0, 2)	(1, 1, 3)			475.2	0.805	Т
[5,-2,-1]	(0, -1, 2)	(1, 1, 3)			475.2	0.805	
[-5,2,-1]	(0, 1, 2)	(-1, -1, 3)			475.2	0.805	Т
[-2,5,1]	(1, 0, 2)	(-1, -1, 3)			475.2	0.805	
[2,-5,-1]	(1, 0, 2)	(-1, -1, 3)			475.2	0.667	I
[-2,-1,-2]	(-1, 0, 1)	(1, -2, 0)			612.8	0.667	
[5,-2,1]	(0, 1, 2)	(-1, -1, 3)			475.2	0.667	Т
[2,1,2]	(-1, 0, 1)	(1, -2, 0)			612.8	0.667	I.
[-5,2,1]	(0, -1, 2)	(1, 1, 3)			475.2	0.667	1
[1,2,2]	(0, -1, 1)	(-2, 1, 0)			612.8	0.667	

FIGURE 18. The possible solutions are provided on a stereographic projection, or tabulated.



FIGURE 19. The number of possible indexing solutions is largely reduced when the microscope parameters (accelerating voltage and camera length) are accurately specified.



FIGURE 20. The comparison of the experimental SAED pattern to a particular solution.



FIGURE 21. Saving the indexing settings using the Keeper dialog.