

Superposition Twinning Supported by Texture - the Showcase of ZnO Nanospikes

Viktor Hrkac[‡], Lorenz Kienle^{*‡}, Sören Kaps[‡], Andriy Lotnyk[†], Yogendra K. Mishra[‡], Ulrich Schürmann[‡], Viola Duppel[§], Bettina V. Lotsch[¶], Rainer Adelung[‡]

SUPPLEMENTARY MATERIAL

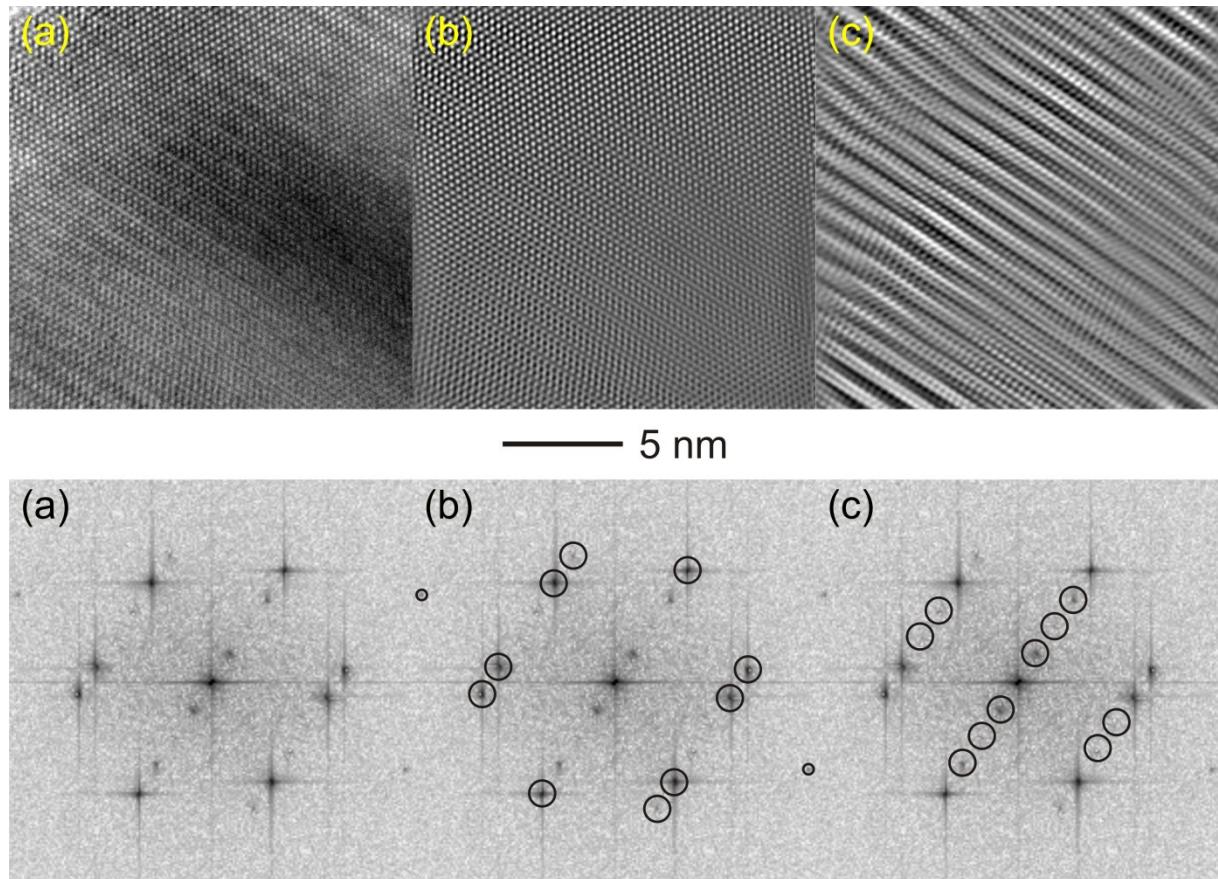


Figure S1: (a) Series of Bragg filtered HRTEM micrographs with associated FFTs:
(a) unfiltered micrograph, (b) filtered micrograph considering only the
fundamental reflections of the two wurtzite domains, (c) filtered micrograph
considering only the satellite reflections.

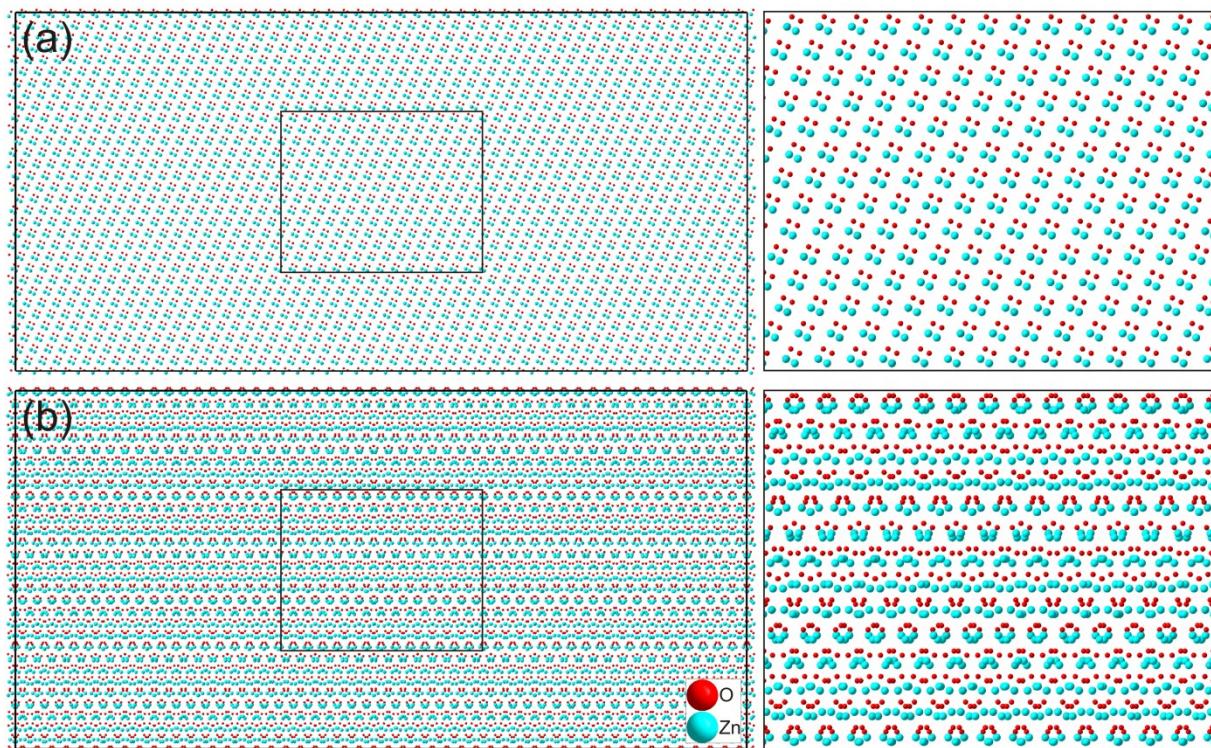


Figure S2. (a) Supercell and (b) superposition structure (SPS) along the $[2 -1 -1 3]^w$ zone axis with enlarged views of the atomic structure.

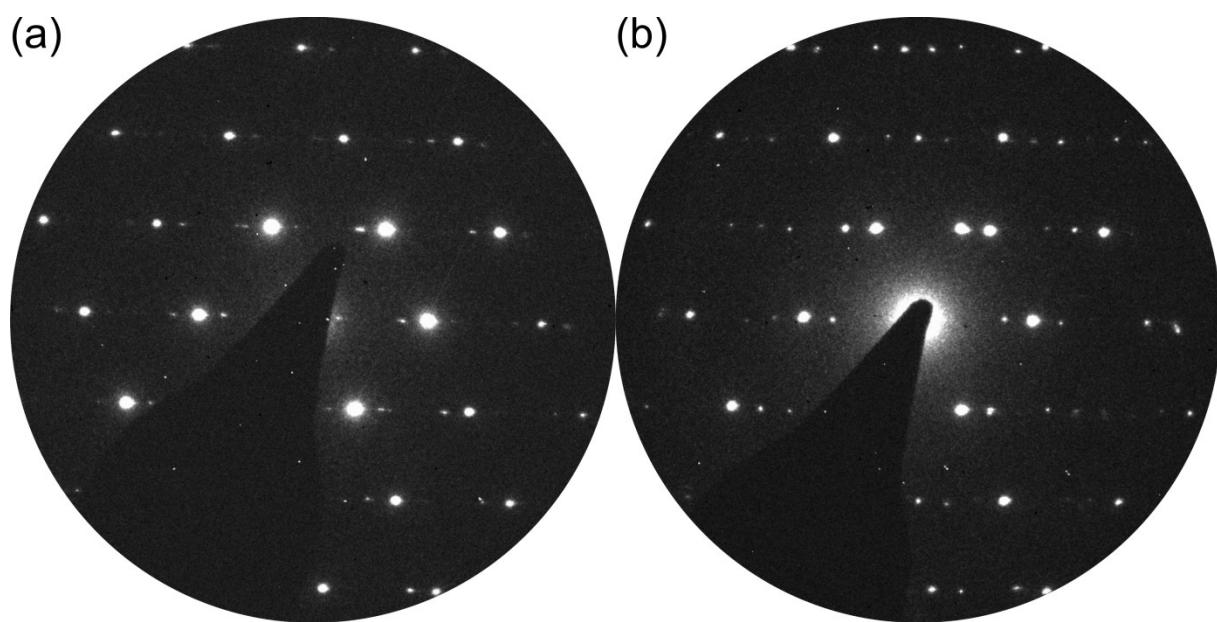


Figure S3. Influence of electron diffraction mode on diffracted intensity. Comparison of (a) SAED and (b) PED patterns of the same area along the $[2 -1 -1 3]^w$ zone axis.

Row No [i]	Reflection	D-Spacing exp. [nm]	D-Spacing theo. [nm]	Twin Domain	Miller Indices [h k i l]
1	a	0.251	0.24755	i	-1 0 1 1
	b	0.286	0.28146	ii	0 -1 1 0
	c	0.316		i+S	-(1/2) -(1/2) 0 (1/2)
	d	0.284	0.28146	i	0 -1 1 0
	e	0.248	0.2476	ii	-1 0 1 1
0	a	0.248	0.24755	ii //	1 -1 0 -1 //
				i	-1 1 0 1
	b	0.334		i+S	-(3/4) (3/4) 0 (3/4)
	c	0.501		i+S	-(1/2) (1/2) 0 (1/2)
	d	0.98		i+S	-(1/4) (1/4) 0 (1/4)
	e	0.98		i+S	(1/4) -(1/4) 0 -(1/4)
	f	0.501		i+S	(1/2) -(1/2) 0 -(1/2)
	g	0.334		i+S	(3/4) -(3/4) 0 -(3/4)
-1	h	0.248	0.24755	ii //	-1 1 0 1 //
				i	1 -1 0 -1
	a	0.248	0.24755	ii	1 0 -1 -1
1	b	0.284	0.28146	i	0 1 -1 0
	c	0.316		i+S	(1/2) (1/2) 0 -(1/2)
	d	0.286	0.28146	ii	0 1 -1 0
	e	0.251	0.24755	i	1 0 -1 -1

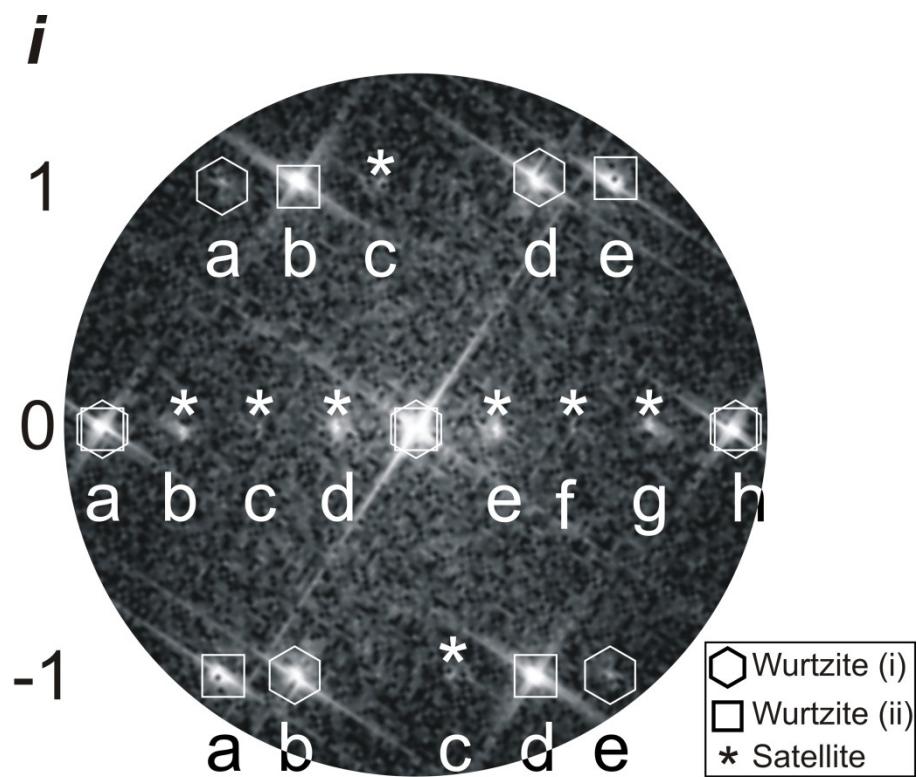


Table S T1. Labeled FFT of Figure 3c-ii. The intensities were separated into two wurtzite type pattern (twin domain **i** and **ii**) and indexed (theoretical d-spacing values and miller indices stem from Sowa, H. (2006). *H. Ahsbahs J. Appl. Crystallography* **39**, p. 169.) Additional satellite intensities were indexed with respect to the twin domain **i** and labeled as **i+S**. The **i** label in the pattern represents the miller index $i = -h-k$.

Row No [l]	Reflection	D-Spacing exp. [nm]	D-Spacing theo. [nm]	Twin Domain	Miller Indices [h k l]
4	a	0.077		i+S	-(9/4) -(7/4) 4 (9/4)
	b	0.077	0.0772 // 0.07756	ii // i	-1 -3 4 1 // -2 -2 4 2
	c	0.077		i+S	-(3/2) -(5/2) 4 (3/2)
	d	0.077		i+S	-(5/4) -(11/4) 4 (5/4)
	e	0.077	0.07756 // 0.0772	ii // i	-2 -2 4 2 // -1 -3 4 1
3	a	0.077	0.07719	ii	1 -4 3 -1
	b	0.089	0.08253	i+S	-(5/2) -(1/2) 3 (5/2)
	c	0.093	0.09382	ii	0 -3 3 0
	d	0.097	0.09848	i	-2 1 3 2
	e	0.102		i+S	-(3/2) -(3/2) 3 (3/2)
	f	0.104	0.10423	ii	-1 -2 3 1
	g	0.104	0.10423	i	-1 -2 3 1
	h	0.101		i+S	-(3/4) -(9/4) 3 (3/4)
	i	0.098	0.09848	ii	-2 -1 3 2
	k	0.093	0.0938	i	0 -3 3 0
	l	0.082	0.08253	ii	-3 0 3 3
	m	0.077	0.07719	i	1 -4 3 -1
2	a	0.077	0.07756	ii	2 -4 2 -2
	b	0.095		i+S	-(11/4) (3/4) 3 (11/4)
	c	0.104	0.10423	ii	1 -3 2 -1
	d	0.113		i+S	-(9/4) (1/4) 2 (9/4)
	e	0.121	0.1238	i	-2 0 2 2
	f	0.140	0.14073	ii	0 -2 2 0
	g	0151	0.15512	i	-1 -1 2 1
	h	0.155		i+S	-(3/4) -(5/4) 2 (3/4)
	i	0.156	0.15512	ii	-1 -1 2 1
	k	0.139	0.1407	i	0 -2 2 0
	l	0.132		i+S	(1/4) -(9/4) 2 -(1/4)
	m	0.122	0.1238	ii	-2 0 2 2
	n	0.112		i+S	(3/4) -(11/4) 2 - (3/4)
	o	0.104	0.10423	i	1 -3 2 -1
	p	0.096		i+S	(5/4) -(13/4) 2 - (5/4)
	q	0.089	0.907	ii	-3 1 2 3
1	a	0.082		i+S	-(13/4) (9/4) 1 (7/4)
	b	0.098	0.09848	ii	2 -3 1-2
	c	0.134	0.13785	i	-2 1 1 2
	d	0.154	0.15512	ii	1 -2 1 -1
	e	0.18		i+S	-(3/2) (1/2) 1 (3/2)
	f	0.243	0.24755	i	-1 0 1 1
	g	0.285	0.28146	ii	0 -1 1 0
	h	0.28	0.28146	i	0 -1 1 0
	i	0.245	0.2476	ii	-1 0 1 1
	k	0.177		i+S	(3/4) -(7/4) 1 -(3/4)
	l	0.154	0.15512	i	1 -2 1 -1
	m	0.135	0.13785	ii	-2 1 1 2

	n	0.121		i+S	(3/2) -(5/2) 1 -(3/2)
	o	0.098	0.0948	i	2 -3 1-2
Row No [i]	Reflection	D-Spacing exp. [nm]	D-Spacing theo. [nm]	Twin Domain	Miller Indices [h k i l]
1	p	0.089	0.0907	ii	-3 1 2 3
0	a	0.075		i+S	-(13/4) (13/4) 0 (13/4)
	b	0.082	0.08253	ii // i	3 -3 0 -3 // -3 3 0 3
	c	0.108		i+S	-(9/4) (9/4) 0 (9/4)
	d	0.123	0.12377	ii // i	2 -2 0 -2 // -2 2 0 2
	e	0.164		i+S	-(3/2) (3/2) 0 (3/2)
	f	0.195		i+S	-(5/4) (5/4) 0 (5/4)
	g	0.246	0.24755	ii // i	1 -1 0 -1 // -1 1 0 1
	h	0.331		i+S	-(3/4) (3/4) 0 (3/4)
	i	0.316		i+S	(3/4) -(3/4) 0 -(3/4)
	k	0.239	0.24755	ii // i	-1 1 0 1 // 1 -1 0 -1
	l	0.193		i+S	(5/4) -(5/4) 0 -(5/4)
	n	0.121	0.12377	ii // i	-2 2 0 2 // 2 -2 0 -2
	o	0.11		i+S	(9/4) -(9/4) 0 -(9/4)
	p	0.088		i+S	(11/4) -(11/4) 0 -(11/4)
	q	0.081	0.08253	ii // i	-3 3 0 3 // 3 -3 0 3
	r	0.075		i+S	(13/4) -(13/4) 0 -(13/4)
-1	a	0.09	0.0907	ii	3 -2 -1 3
	b	0.098	0.09846	i	-2 3 -1 2
	c	0.136	0.13785	ii	2 -1 -1 -2
	d	0.154	0.15512	i	-1 2 -1 1
	e	0.177		i+S	-(3/4) (7/4) -1 (3/4)
	f	0.271	0.28146	ii	0 1 -1 0
	g	0.235	0.24755	i	1 0 -1 -1
	h	0.174		i+S	(3/2) -(1/2) -1 -(3/2)
	i	0.151	0.15512	ii	-1 2 -1 1
	k	0.132	0.13785	i	2 -1 -1 -2
	l	0.106		i+S	(5/2) -(3/2) -1 -(5/2)
	m	0.096	0.09848	ii	-2 3 -1 2
	n	0.08		i+S	(13/4) -(9/4) -1 -(13/4)
-2	a	0.077	0.07755	i	-2 4 -2 2
	b	0.09	0.0907	ii	3 -1 -2 -3
	c	0.096		i+S	-(5/4) (13/4) -2 (5/4)
	d	0.152		i+S	(3/4) (5/4) -2 -(3/4)
	e	0.148	0.15512	i	1 1 -2 -1
	f	0.137	0.14073	ii	0 2 -2 0
	g	0.118	0.12377	i	2 0 -2 -2
	h	0.111		i+S	(9/4) -(1/4) -2 -(9/4)

	i	0.102	0.104	ii	-1 3 -2 1
	k	0.82		i+S	(13/4) -(5/4) -2 -(13/4)
	l	0.076	0.07756	ii	-2 4 -2 2
-3	a	0.074		i+S	-(5/4) (17/4) -3 (5/4)
	b	0.102	0.104	ii	1 2 -3 -1
Row No [i]	Reflection	D-Spacing exp. [nm]	D-Spacing theo. [nm]	Twin Domain	Miller Indices [h k l]
-3	c	0.1		i+S	(3/2) (3/2) -3 -(3/2)
	d	0.097	0.09848	i	2 1 -3 -2
	e	0.092	0.9382	ii	0 3 -3 0
	f	0.087		i+S	(5/2) (1/2) -3 (5/2)
	g	0.076	0.07719	ii	-1 -4 -3 1
-4	a	0.074		i+S	(7/4) (9/4) -4 -(7/4)
	B	0.076	0.0772// 0.07756	ii // i	1 3 -4 -1 // 2 2 -4 -2
	c	0.074		i+S	(9/4) (7/4) -4 -(9/4)
	D	0.07	0.07036 // 0.07119	ii // i	0 4 -4 0// 3 1 -4 -3

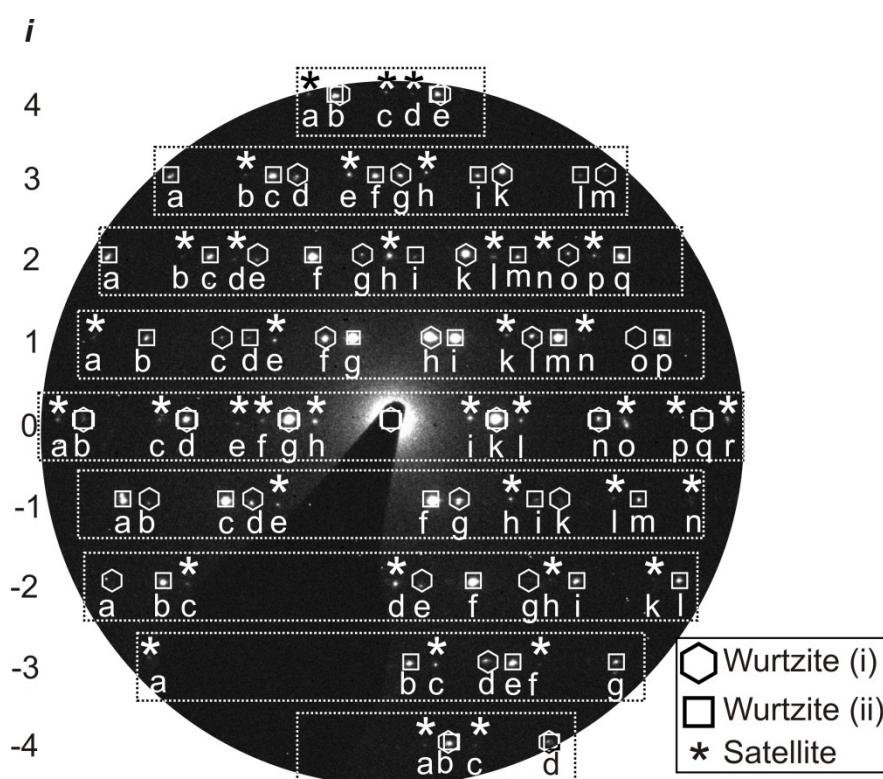


Table S T2. Experimentally obtained PED pattern along the zone axis [2 -1 -1 3]. The reflections were separated into two wurtzite type pattern (twin domain **i** and **ii**) and indexed (theoretical d-spacing values and miller indices stem from Sowa, H. (2006). *H. Ahsbahs J. Appl. Crystallography* **39**, p. 169.) Additional satellite

reflections were indexed with respect to the twin domain \mathbf{i} and labeled as $\mathbf{i}+\mathbf{S}$.
The \mathbf{i} label in the pattern represents the miller index $\mathbf{i} = -h-k$.