Electronic Supplementary Information

Graphene/SiC Heterojunction Nanoarrays: Toward Field Emission Applications with Low Turn-on fields and High Stabilities

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Table 1 Turn-on fields[a], highest current density and the corresponding applied external fields, field enhancement factors (β), and current emission stability (current density, testing time and current fluctuation) for SiC nanostructured field emitters, other typical nanostructured emitters, as well as other commonly used emitters.

	SiC field emitters	E_{to} (V/μm)	Highest current density (mA/cm^2) and the applied fields (V/μm)	β	Current stability (current density, time, fluctuations)	Ref.
SiC nanostructured emitters	**B-doped G/SiC heterojunction nanoarrays**	**1.10-1.12**	**8.2** **1.85**	**6384**	**662.5 μA/cm^2, 5 h, 3.7%**	**This work**
	Patterned SiC nanowire arrays	1.54	~0.22 ~2.2	4248	--, --, --	1
	SiC quasi-aligned nanoneedle arrays	1.4-3.4	~1.5 ~1.22	--	~200 μA/cm^2, 10 h, --	2
	Au-decorated SiC nanowires	1.14	~3.8 ~2.1	6244	--, --, --	3
	P-doped SiC nanoparticles	1.03	~4.6 ~1.8	5508	2.65 mA/cm^2, 20 h, ±2.1-3.4%	4
	Carbon decorated SiC nanowires	0.5	~14 ~2.3	--	2.0 mA/cm^2, 2 h, $<$ 5%	5
	N-doped SiC nanoneedles	1.11	~3.4 ~1.68	--	1.138 mA/cm^2, 1 h, 8.1%	6
	B-doped SiC nanoneedle arrays	1.92	~1.4 ~3.98	3643	512.9 μA/cm^2, 8 h, 6.5-7.8%	7
	n-type β-SiC nanoarrays	1.57-1.95	~2.3 ~2.43	3217-3340	--, --, --	8
	Well-aligned SiC nanowires arrays	1.50	~2.3 ~2.98	4482	693.3 μA/cm^2, 4 h, $<$ 3.8%	9
	B-doped 3C-SiC nanowires	1.35	~1.4 ~2.57	4895	--, 10 h, 11-14%	10
	N-doped SiC nanoneedles	1.37	~3.5 ~1.06	2486	--, 1 h, 7.7%-14.1%	11
	N-doped nanoporous SiC	4.4-9.6	6 A/cm^2 ~7.5	936-3636	--, --, --	12
	N-doped SiC nanoarrays	1.9-2.65	~2.1 ~2.62	1710	--, --, --	13
	N-doped 3C-SiC nanoneedles	~1.1	~5.0 ~2.2	6500	1.7 mA/cm^2, 0.5 h, --	14
	Tapered SiC nanowires	1.2	~0.6 ~1.99	3368	--, --, --	15
	Al_2O_3-decorated tubular SiC	2.4	~10.0 ~5.0	--	--, --, --	16
	Aligned SiC porous nanowires	2.3-2.9	~2.3 ~7.96	5241	570 μA/cm^2, 20 h, --	17
	β-SiC nanowires	--	--	2000	--, --, --	18
	β-SiC nanoarchitectures	12	~0.035 --	--	--, --, --	19
	SiC nanowires/nanorods	3.33	--	--	--, --, --	20
	Nonaligned SiC nanowires	3.1-3.5	~0.09 ~6.05	--	60 μA/cm^2, 2 h , ±15%	21
	Vertical carbon nanotubes	0.4-1.1	~1.2 ~0.7	9000-14500	~500 μA/cm^2, 158 h, --	22

Other typical inorganic nanostructured emitters	Carbon nanotubes arrays	--	~10 --	--	500 μA/cm^2, 20 h, --	23
	Carbon nanotubes	3.6	--	1112-1546	--, --, --	24
	Multiwall carbon nanotubes	2.05 (1 μA/cm^2)	~0.06 ~2.3	1023, 16434	--, 10 h, --	25
	Aligned untralong ZnO nanobelts	1.3	~1.2 ~3.0	14000	--, --, --	26
	Ultrathin ZnO nanobelts	--	~40 ~11	700	7.4 mA/cm^2, 16 h, ~14%	27
	Vertical ZnO nanowires/graphene	2.0-2.8	~0.9 ~2.9	3834-6473	--, --, --	28
	Single-layer graphene films	2.3	~22 ~6.1	3700	11.46 mA/cm^2, 12 h, ~4%	29
	Graphene nanosheets	2.04	~1.2 ~3.3	--	~700 μA/cm^2, 12 h, --	30
	Si-doped AlN nanoneedle array	1.8	~22 ~5.4	3271	10 mA/cm^2, 5 h, ＜ 5%	31
	Aligned AlN nanorods	3.8	~7 ~8.4	950	--,--,--	32
	AlN nanorod arrays	4.7	~24 ~22	1175.5 - 1888.7	--, 4 h, 0.74%	33
	Ultrafine ZnS nanobelts	3.47	~12 ~5.5	2000	--,--,--	34
	ZnS nanobelts arrays	3.8	~0.035 ~4.3	1839	--,--,--	35
	Single-crystalline PrB_6 nanorods	0.95-2.8	~13 ~7.25	823-1390	250 μA/cm^2, ~17 h, ＜10%	36
	Single-crystalline LaB_6 nanowires	1.06-1.82	~6.0 ~2.85	1072	~500 μA/cm^2, ~17 h, ＜6.0%	37
	CeB_6 nanorods	1.8	~0.013 ~12	1035-3863	12.8 μA/cm^2, 3 h, 1.41-1.51%	38
	SmB_6 nanowires	2.7-4.2	~10 ~9.7	2207-4741	--, 500 min, 10%	39
	SnO_2 nanowires	3.5	~6.5 ~7.5	1225	~1 mAcm^{-2}, 40 h, --	40
	Single-crystalline CdS nanobelts	3.7	~3.7 ~11	1298	~200 μA/cm^2, 75 h, 5%	41
	Tungsten oxide nanowires	--	~12 ~4.65	1657	5.25 mA/cm^2, 1 h, ~5%	42
	Oriented CuO nanoknife arrays	0.9	~1.6 ~1.25	2400-5400	1.15 mA/cm^2, ~1 h, ~5%	43

[a] The turn-on field is defined to the electric field required to generate an emission current density of 10 μA/cm^2. If other values are used, it will be mentioned separately.

Calculation on Electronic Band Structures

The electronic band structures of the pure and B-doped SiC nanowires are calculated based on the VASP code[44] and density functional theory (DFT) with the exchange-correlation functional of Perdew, Burke, and Ernzerhof revised for solids (PBEsol).[45] The numbers of the valence electrons for C, Si and B atoms included in the calculations are 4, 4 and 5 respectively. The valence wave functions are expanded in a plane wave basis with a cutoff energy of 330 eV. A 4×4×8 grid is applied for the *K*-point mesh sampling the Brillouin zone. Further increasing the energy cutoff and *K*-points exhibit little difference in the results. All the structures considered in this study have been fully relaxed with a conjugate-gradient algorithm until the energy on the atoms is less than 1.0×10^{-4} eV. Meanwhile, the periodic boundary conditions have been applied in all three dimensions. As an example, in current calculation, the concentration of B dopant is roughly set as 2.6 *at.*%, which is about half to that of the experimental setup for qualitatively reflecting the electronic structures of pure and B-doped 3*C*-SiC samples. Several supercells of B-doped 3*C*-SiC with B occupying unequivalent Si sites have been examined. The calculations disclose that, as compared to that of the pure counterpart, the B dopants doped into the SiC nanowires *via* the formation of substitutional solid solutions might favor a more localized state near the Fermi energy level. This could facilitate a more facile electron excitation from the valence band to the vacuum level, consequently leading to the remarkable enhancement on the FE properties of G/SiC heterojunction nanowire arrays.

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