

Supplemental Information

Breakdown Current Density in BN-Capped Quasi-1D TaSe₃ Metallic Nanowires: Prospects of Interconnect Applications

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I. Materials Characterization

The samples for x-ray diffraction (XRD) were prepared by grinding TaSe₃ crystals in a mortar and pestle before pressing into an aluminum mount. Data were collected on a Bruker D8-Advance (Co-K α radiation) diffractometer from 10-80 2θ at a rate of 0.1 s per step at 40 mA,

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40 kV. For SEM/EDS and EPMA analyses, crystals were mounted on double-sided carbon tape. SEM images were acquired with an FEI Inspect F field emission gun scanning electron microscope operated at 20 keV, with an EDAX energy dispersive spectroscopy attachment. EPMA data were collected with a JEOL JXA 8600 Superprobe instrument.

II. Optical Microscopy

High-quality TaSe₃ crystals were prepared by the chemical vapor transport (CVT) method using iodine. Figure S1 is an optical microscopy image of the synthesized TaSe₃ crystals before chemical and mechanical exfoliation.

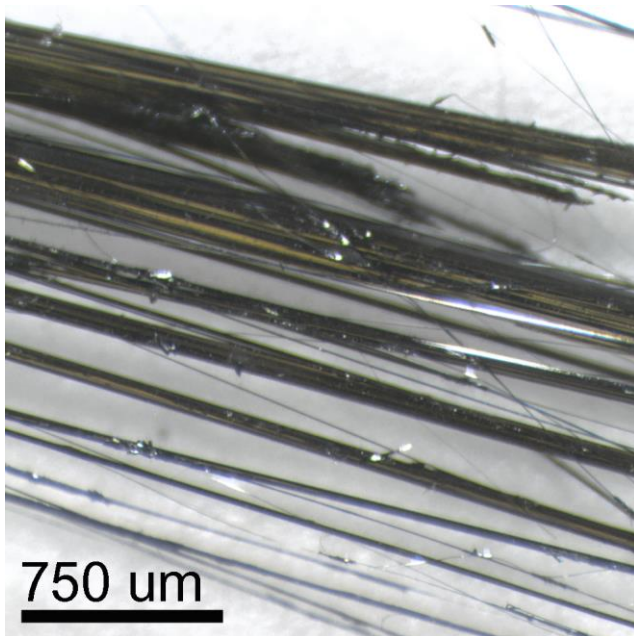


Figure S1: Optical microscopy image of TaSe₃ crystals.

III. Transmission Electron Microscopy

Transmission electron microscopy and electron diffraction were performed on a FEI Tecnai12 TEM at the Central Facility for Advanced Microscopy and Microanalysis at UC Riverside.

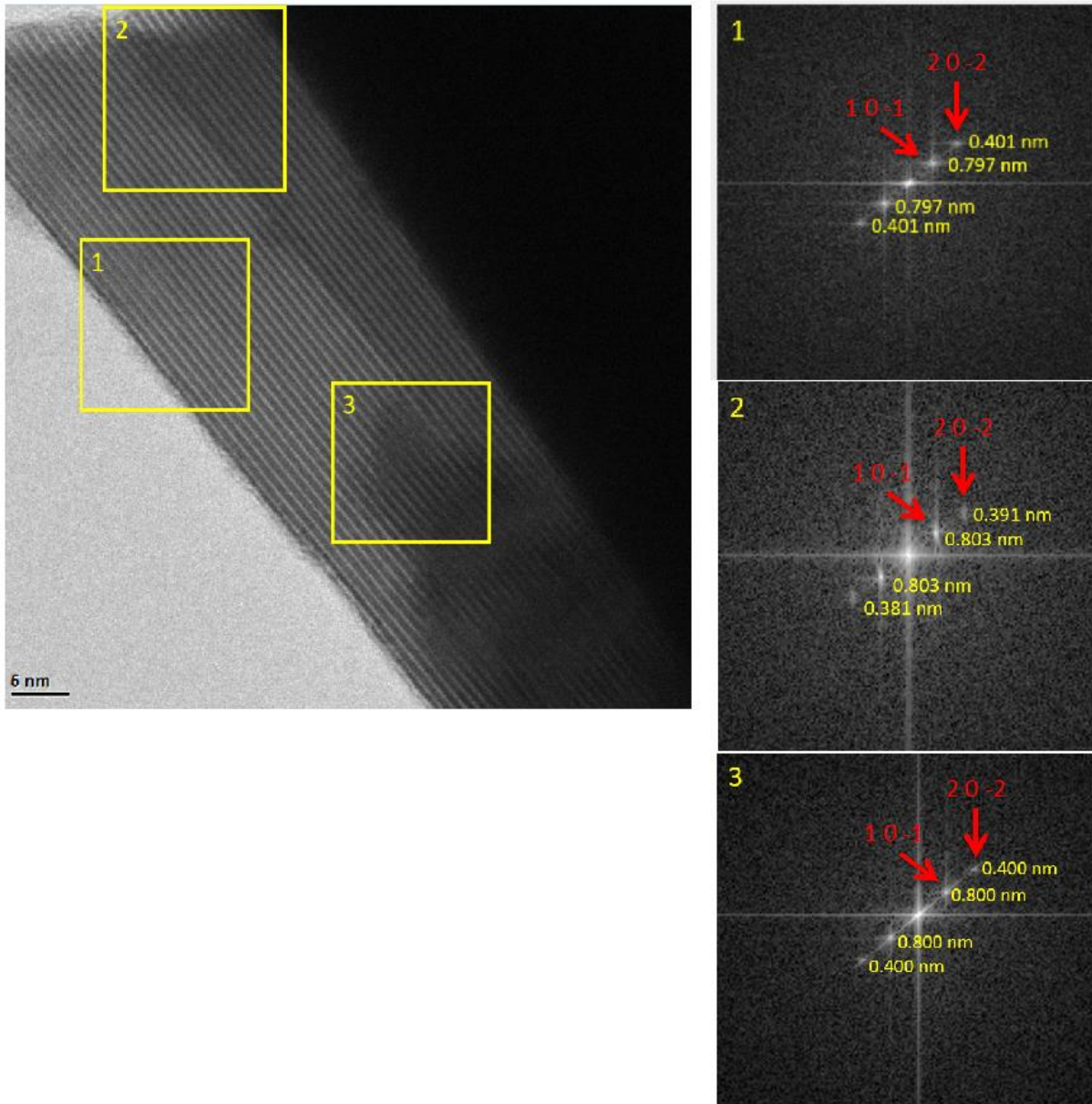


Figure S2: FFT analysis for the HRTEM image in Figure 1(c). Spots were matched using d-spacing values for the monoclinic TaSe₃ structure (below).

Table S1: Values for the d-spacing of the monoclinic TaSe₃ structure.

monoclinic TaSe ₃					
d-spacing[Å]	2θ	rel. I [%]	h	k	l
9.9859	8.848	3.15	1	0	0
9.4358	9.365	8.85	0	0	1
8.0801	10.941	100.00	1	0	-1
6.0631	14.598	1.87	1	0	1
5.0342	17.603	20.60	2	0	-1
4.9930	17.750	32.57	2	0	0
4.8186	18.398	34.57	1	0	2
4.71793	18.7924	14.93	0	0	2
4.04007	21.9818	2.60	2	0	-2
3.97683	22.3358	4.06	2	0	1
3.86795	22.9730	29.93	1	0	2
3.45741	25.7450	13.02	3	0	-1
3.32864	26.7591	0.09	3	0	0
3.29879	27.0058	0.16	1	1	0
3.27740	27.1854	0.96	0	1	1
3.27416	27.2128	0.13	1	0	-3
3.20778	27.7871	4.55	-1	1	1
3.16988	28.1262	1.48	3	0	-2
3.14528	28.3507	4.40	0	0	3
3.07820	28.9820	0.27	2	0	-3
3.03154	29.4380	1.89	2	0	2
3.02795	29.4737	7.74	1	1	1
2.89503	30.8598	2.40	3	0	1
2.87095	31.1252	0.52	-2	1	1
2.86324	31.2112	5.52	2	1	0
2.82917	31.5968	97.78	-1	1	2
2.80836	31.8370	3.79	0	1	2
2.78487	32.1129	0.04	1	0	-3
2.69338	33.2348	0.17	3	0	-3

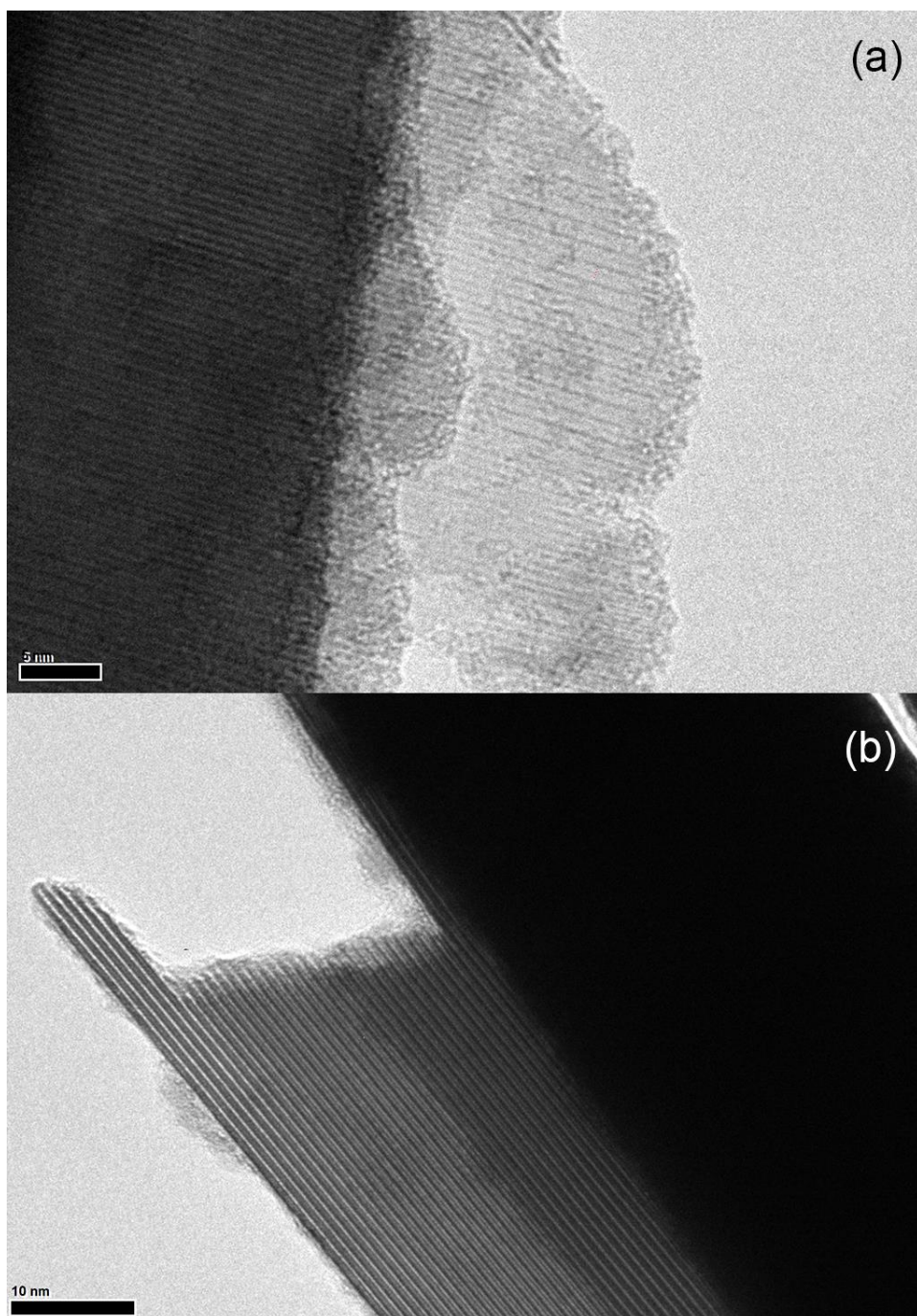


Figure S3: Additional TEM images of quasi-1D TaSe₃ nanowires after chemical exfoliation.

IV. Analysis of Elemental Composition

Table S2: Data on the elemental composition of CVT-grown TaSe₃ crystals are summarized below.

	Theoretical weight %	Experimental weight %		Theoretical atomic %	Experimental atomic %	
		EPMA	EDS		EPMA	EDS
Se	56.70	55.12	54.94	75.00	73.47	74.08
Ta	43.30	43.13	45.06	25.00	26.53	25.92
Total						
weight %	100.0	98.25	100.0	-	-	-
Se/Ta	-	-	-	3.00	2.77	2.86

V. Atomic Force Microscopy

Figure S4 illustrates AFM characterization of the current breakdown point in TaSe₃ nanowire.

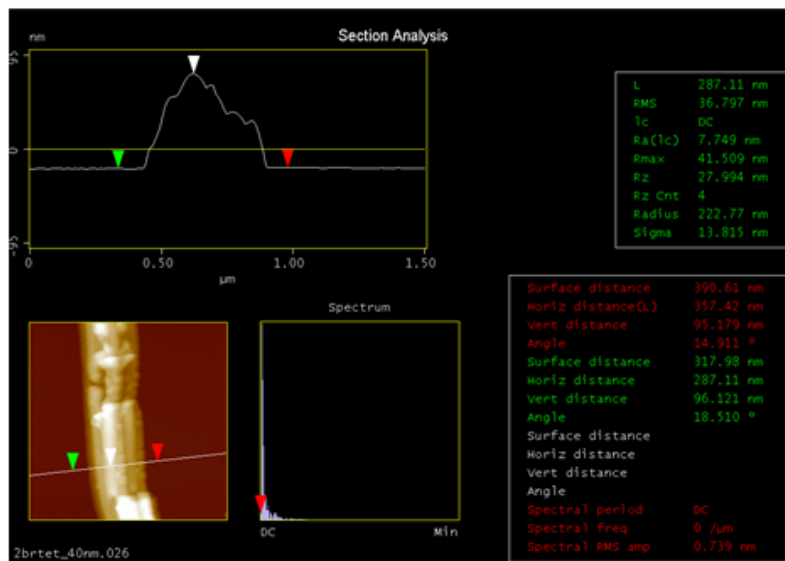


Figure S4: Representative AFM image of the breakdown point in TaSe₃ nanowire.

VI. Device Fabrication

In order to prevent material oxidation, TaSe₃ nanowires were capped immediately after being mechanically exfoliated. The fabricated heterostructures were spin coated with a positive resist polymethyl methacrylate (PMMA) and heated two times. Patterning of the assembled stacks was accomplished by electron beam lithography (EBL) (LEO Supra). In order to expose TaSe₃ material covered by h-BN, the assembled stacks were selectively etched with sulfur hexafluoride (SF₆) gas on an inductively coupled plasma system (Oxford Plasmalab). Time of ICP treatment with 50 sccm of SF₆ varied from 20 sec to 180 sec depending on hBN thickness and each time was adjusted gradually. Total of about fifty h-BN capped and not capped prototypes were fabricated within the scope of this work. Optical microscopy image in Figure S5 show a representative h-BN capped TaSe₃ nanowire device.

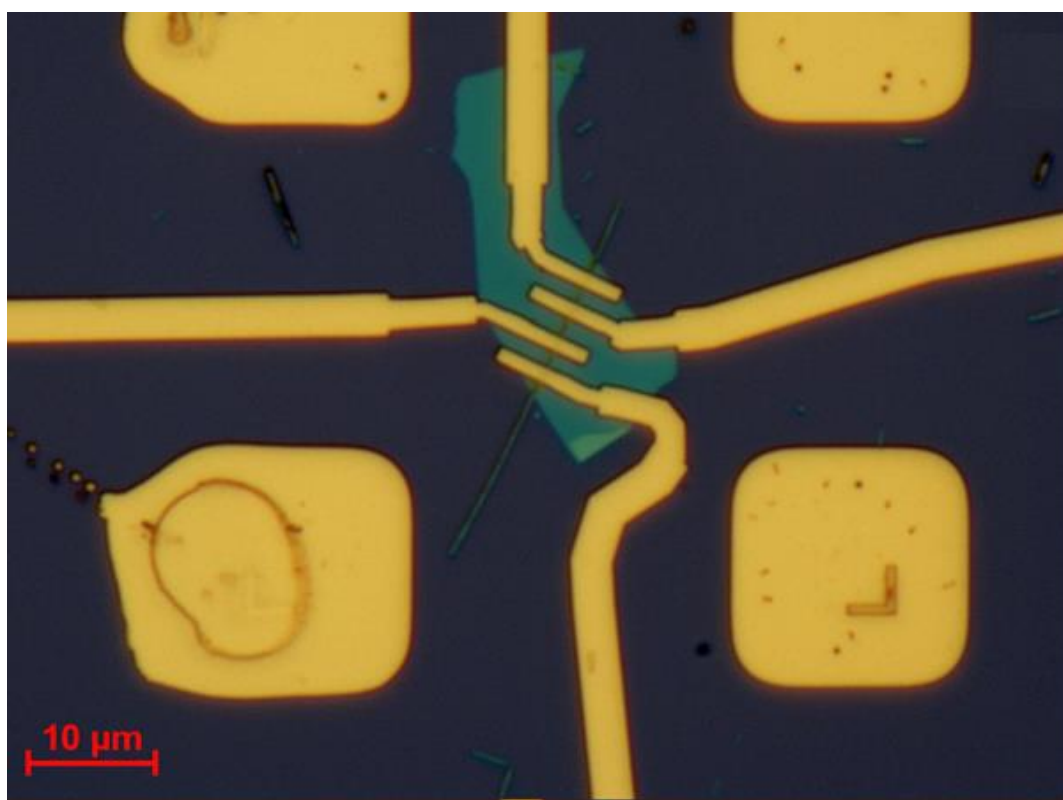


Figure S5: Optical microscopy images of quasi-1D TaSe₃ nanowire capped with h-BN layer.

VII. Scanning Electron Microscopy

The SEM inspection confirmed significantly lower roughness of a TaSe₃ metallic nanowires in comparison with the deposited metal contacts (see Figure S6). Roughness estimated by AFM was in the range from 0.2 nm to 0.5 nm.

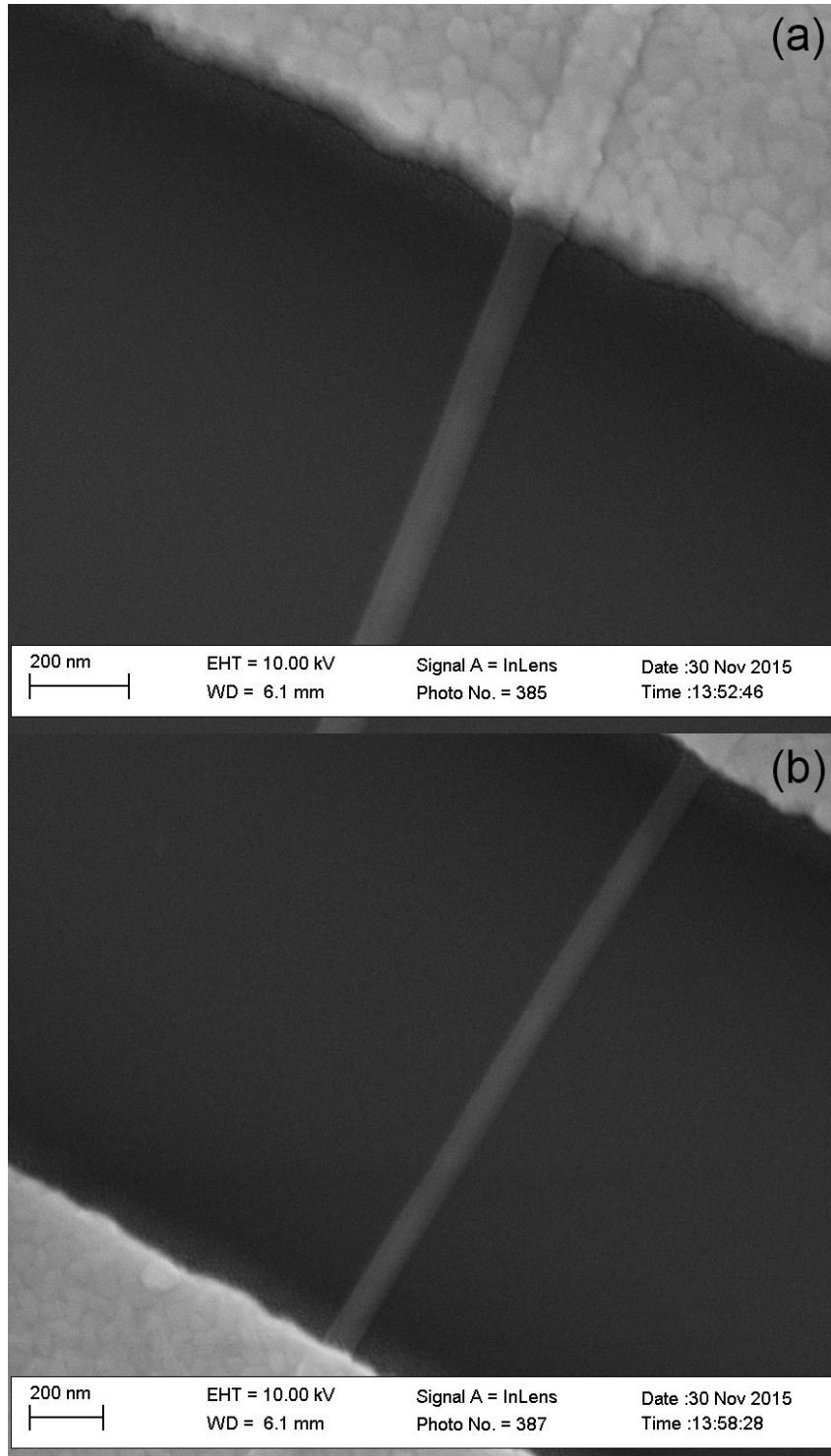


Figure S6: SEM images of representative quasi-1D TaSe₃ nanowires.