Electronic Supplementary Material (ESI) for Nanoscale.

Supplemental Information

Unique Features of the Generation–Recombination Noise in Quasi-One-Dimensional Van der Waals Nanoribbons

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CVT crystal growth of $ZrTe_3$: A 17.78 × 1 cm fused quartz ampule (cleaned overnight in nitric acid, followed by 12 h at 900 °C) was charged with zirconium foil (4.23 mmol, Sigma-Aldrich 99.98% purity), tellurium powder (12.7 mmol, Sigma-Aldrich 99.8% purity), and iodine crystals (~4.5 mg cm^{-3}, J. T. Baker, 99.9% purity). The ampule was evacuated and backfilled with Ar 3× while submerged in a cold bath. After flame sealing, the ampule was placed in a two-zone horizontal tube furnace and heated at 10 °C min^{-1} to a final temperature gradient of 850–750 °C that was held for 7 days. After cooling to room temperature and removing excess iodine under vacuum, silver-black, platelet crystals of $ZrTe_3$ were isolated (Figure S1).

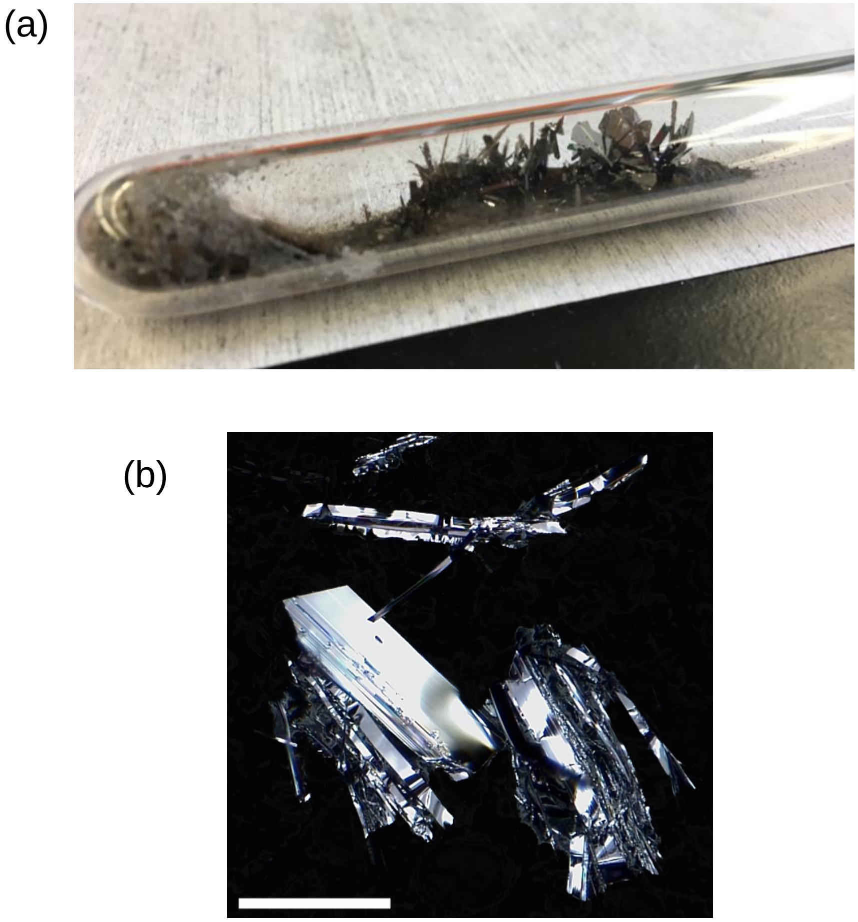

Figure S1: (a) CVT growth ampule containing $ZrTe_3$ crystals. (b) Optical microscopy image of several isolated $ZrTe_3$ crystals (scale bar = 500 μm)

Experimental details for the single crystal x-ray diffraction structure determination of $ZrTe_3$: Data collection: A dark-silver crystal was mounted on a tip of a glass fiber. The X-ray intensity data were measured at room temperature on a Bruker D8 Quest PHOTON 100 CMOS X-ray diffractometer system with Incoatec Microfocus Source (IμS) monochromated Mo Kα radiation (λ = 0.71073 Å, sealed tube) using phi and omega-scan technique. The data were collected in 2920 frames with 10 second exposure times. Crystallographic data are summarized in Table S1.

Data reduction: Of the 939 unique reflections collected, 937 were observed ($I > 2\ \sigma(I)$). The linear absorption coefficient for Mo Kα radiation is 20.688 mm^{-1}. The data were corrected for Lorentz and polarization effects and integrated with the manufacturer's SAINT software. Absorption corrections were applied with the multi-scan method (SADABS).[S1]

Structure solution and refinement: Subsequent solution and refinement was performed using the SHELXTL-2014 solution package operating on a Pentium computer.[S2,S3] The structure was solved by intrinsic phasing method using SHELXTL-2014 Software Package. Non-hydrogen atomic scattering factors were taken from the literature tabulations,[S4] and the real and imaginary anomalous dispersion corrections were those of Cromer.[S5] Non-hydrogen atoms were located from successive difference Fourier map calculations. In the final cycles of each refinement, the all atoms were refined in anisotropic displacement parameters. The crystal system of compound is monoclinic, space group P2(1)/m (No. 11) and the final residual values based on 26 variable parameters and 937 observed reflections ($I > 2\ \sigma(I)$) are $R1 = 0.0200$, $wR2 = 0.0610$, and those for all unique reflections are $R1 = 0.0201$, $wR2 = 0.0611$. The goodness-of-fit indicator for all data is 1.004. Peaks on the final difference map, ranging from 1.890 to –2.329 $e/Å^3$ around Te(3) (0.67 Å from Te(3)) and Te(3) (1.51 Å from Te(3)) atoms, are of no chemical significance.

Table S1: Summary of crystallographic data

	$ZrTe_3$
Formula	$ZrTe_3$
F.W. (g/mol)	474.02
Space group	$P2_1/m$
Z	2
a (Å)	5.8938(3)
b (Å)	3.9256(2)
c (Å)	10.1011(5)
β (°)	97.8200(10)
V (Å^3)	231.53(2)
Absorption coefficient	Numerical
μ (mm^{-1})	20.688
θ range (deg.)	3.489–32.577
hkl ranges	$-8 \leq h \leq 8$ $-5 \leq k \leq 5$ $-15 \leq l \leq 15$
No. reflections; R_{int}	939; 0.0308
No. parameters	26
R_1; wR_2	0.0201; 0.0611
Goodness of Fit	1.004
Diffraction peak and hole (e$^-$/Å^3)	1.890; –2.329
Temperature (K)	297(2)

Table S2: Atomic coordinates for $ZrTe_3$ with equivalent isotropic displacement parameters (Å^2). U_{eq} is defined as 1/3 of the orthogonalized trace of the *Uij* tensor.

		$ZrTe_3$		
Atom	x	y	z	U_{eq}
Zr1	2883(1)	7500	6657(1)	6(1)
Te1	2364(1)	12500	4448(1)	7(1)
Te2	5674(1)	2500	8326(1)	10(1)
Te3	952(1)	2500	8391(1)	10(1)

Table S3: Bond lengths [Å] for $ZrTe_3$

Zr(1)-Te(2)#1	2.9398(4)
Zr(1)-Te(2)	2.9399(4)
Zr(1)-Te(1)#2	2.9564(4)
Zr(1)-Te(1)	2.9564(4)
Zr(1)-Te(3)	2.9593(4)
Zr(1)-Te(3)#1	2.9593(4)
Zr(1)-Te(1)#3	3.1422(5)
Zr(1)-Te(1)#4	3.1532(5)
Zr(1)-Zr(1)#2	3.9256(2)
Zr(1)-Zr(1)#5	4.8496(8)
Zr(1)-Zr(1)#6	4.8540(8)
Te(1)-Zr(1)#1	2.9565(4)
Te(1)-Zr(1)#3	3.1421(5)
Te(1)-Zr(1)#4	3.1533(5)
Te(1)-Te(1)#3	3.7026(5)
Te(1)-Te(2)#6	3.7312(4)
Te(1)-Te(3)#5	3.7912(4)
Te(1)-Te(1)#2	3.92560(19)
Te(2)-Te(3)	2.7923(4)
Te(2)-Zr(1)#2	2.9399(4)
Te(2)-Te(3)#7	3.1030(4)
Te(2)-Te(2)#2	3.9256(2)
Te(2)-Te(2)#8	4.0809(6)
Te(2)-Te(3)#8	4.1244(4)
Te(3)-Zr(1)#2	2.9593(4)
Te(3)-Te(2)#9	3.1030(4)
Te(3)-Te(3)#2	3.9256(2)
Te(3)-Te(3)#10	4.0829(6)

Table S4: Anisotropic displacement parameters (A^2 x 10^3) for $ZrTe_3$. The anisotropic displacement factor exponent takes the form: -2 pi^2 [h^2 a*^2 U11 + ... + 2 h k a* b* U12]

	U11	U22	U33	U23	U13	U12
Zr(1)	7(1)	6(1)	6(1)	0	1(1)	0
Te(1)	7(1)	8(1)	5(1)	0	1(1)	0
Te(2)	7(1)	11(1)	11(1)	0	0(1)	0
Te(3)	9(1)	11(1)	12(1)	0	5(1)	0

References:

S1. Data Reduction:

Intensity

$$I = [S - B/R]\cdot V$$

Standard Deviation in Intensity

$$s(I) = [S + B/R^2]^{1/2}\cdot V$$

Structure Factor

$$F = (I/Lp)^{1/2}$$

Standard Deviation in Structure Factor

$$\sigma(F) = \sigma(I)/(2\cdot F\cdot Lp)$$

Where:
S = total scan count
B = sum of background counts
R = ratio of background counting time to scan counting time
V = scan rate
Lp = Lorentz-polarization correction

S2. Least-Squares Refinement:

Weighting Scheme

$$w = 1/[\sigma^2(F_o^2) + 0.0455*P)^2 + 1.2493*P] \text{ where } P = [\mathrm{Max}(F_o^2, 0) + 2*F_c^2]/3;$$

Residuals

R-factors:

$$R = \Sigma \big| |F_o| - |F_c| \big| / \Sigma |F_o|;$$

Weighted R-factor on F^2:

$$wR2 = [\Sigma[w(F_o^2 - F_c^2)^2] / \Sigma[w(F_o^2)^2]]^{1/2};$$

Goodness of Fit Indicator:

$$\text{goodness-of-fit} = [\Sigma[w(F_o^2 - F_c^2)^2] / (N_{observns} - N_{params})]^{1/2}.$$

S3. (a) Sheldrick, G.M. *SHELXTL-2014*, *Crystallographic Computing System*; Bruker Analytical X-Ray Instruments: Madison, WI, 2014; (b) Sheldrick, G.M. *A Short History of SHELX*, Acta Cryst. 2008, A64, 112.

S4. Cromer, D.T. and Waber, J.T. International Tables for X-ray Crystallography, Vol. IV, Table 2.2B, The Kynoch Press, Birmingham England, 1974.

S5. Cromer, D.T. International Tables for X-ray Crystallography, Vol. IV, Table 2.3.1, The Kynoch Press, Birmingham England, 1974.

EDS analysis of $ZrTe_3$:

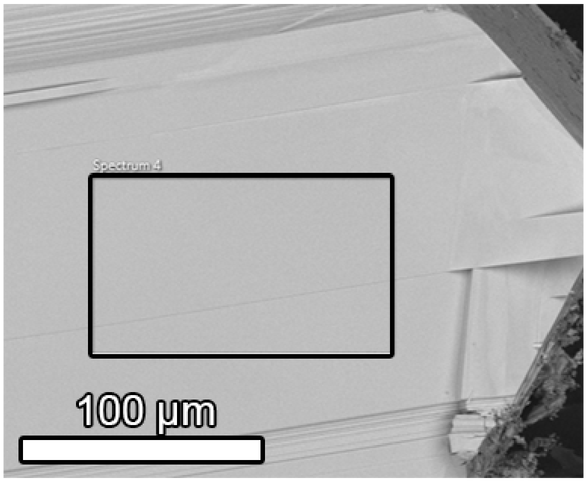

Figure S2: SEM (backscatter mode) of a CVT-grown $ZrTe_3$ crystal; its surface was removed by mechanical exfoliation prior to EDS characterization.

Table S5: Experimental and theoretical atomic % for a representative CVT-grown $ZrTe_3$ crystal; the experimental data is averaged over a relatively flat area of the crystal (the boxed region shown in Figure S2).

	Zr Atomic %	**Te Atomic %**
Experimental	26.3	73.8
Theoretical	25.0	75.0