Low Resistivity and High Breakdown Current Density of 10-nm Diameter van der Waals $TaSe_3$ Nanowires by Chemical Vapor Deposition

Thomas A. Empante[1], Aimee Martinez[1], Michelle Wurch[1], Yanbing Zhu[2], Adane K. Geremew[3], Koichi Yamaguchi[1], Miguel Isarraraz[1], Sergey Rumyantsev[3,4], Evan J. Reed[2], Alexander A. Balandin[3], Ludwig Bartels[1]

[1]Department of Chemistry and Material Science & Engineering Program, University of California – Riverside, Riverside, CA 92521, United States

[2]Department of Materials Science and Engineering, Stanford University, Stanford, California 94304, United States

[3]Nano-Device Laboratory, Department of Electrical and Computer Engineering, University of California, Riverside, California 92521, United States

[4]Center for Terahertz Research and Applications, Institute of High Pressure Physics, Polish Academy of Sciences, Warsaw 01-142, Poland

Supporting Information

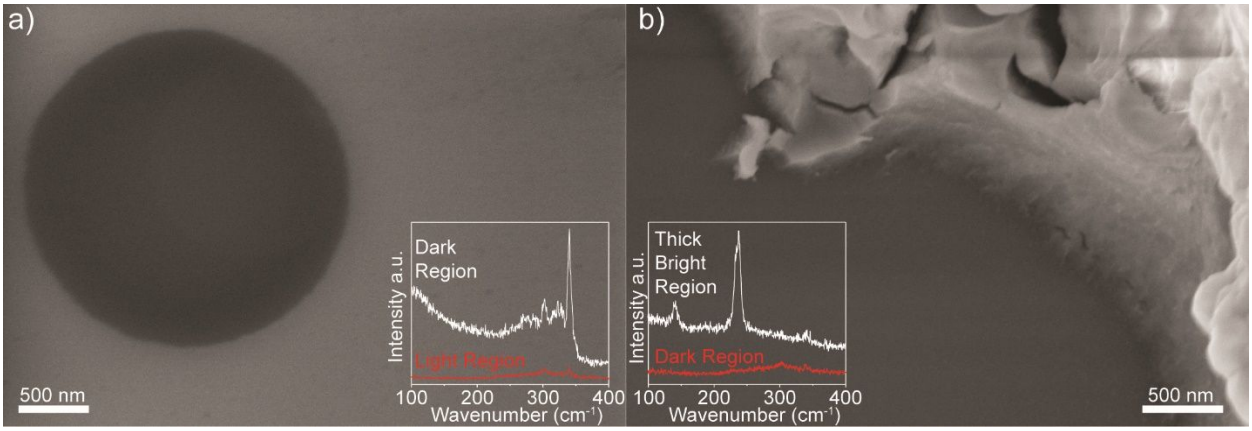

Figure S1: Scanning electron microscopy images and Raman spectra (on and off precipitate) for drops of the following solutions dried on a 300nm SiO_2/Si substrate: a) $TaCl_5$ mixed with diethyl ether and b) $TaCl_5$ mixed with diethyl ether and dissolved in ethanol. Both a) and b) lack any nanowire structures in the SEM. Neither of the precipitates exhibit the Raman signature seen for the $TaSe_3$ nanowires. The Raman peaks at 141 and 237cm^{-1} after addition of both diethyl ether and ethanol, b), resemble those of 2H $TaSe_2$.

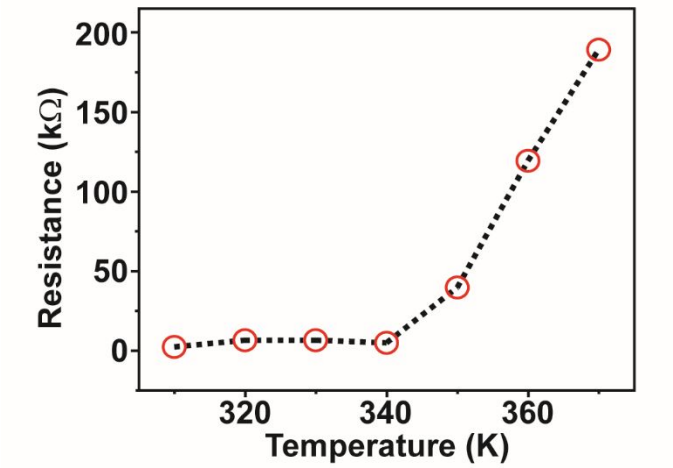

Figure S2: Resistance of a CVD 1D vdW $TaSe_3$ nanowire bundle as a function of temperature. The resistivity increases with temperature, similar to other metals. The gradual and relatively slow resistance increase below 350 K is due to increasing electron−phonon scattering. The sharp increase in resistance at temperatures above 350 K is likely related to the onset of electromigration as commonly observed in conventional interconnect reliability tests.[1-4] The slope may be enhanced by local self-heating due to the small wire bundle cross section area and low thermal conductivity of the SiO_2 layer under the nanowire and PMMA film encapsulating it.

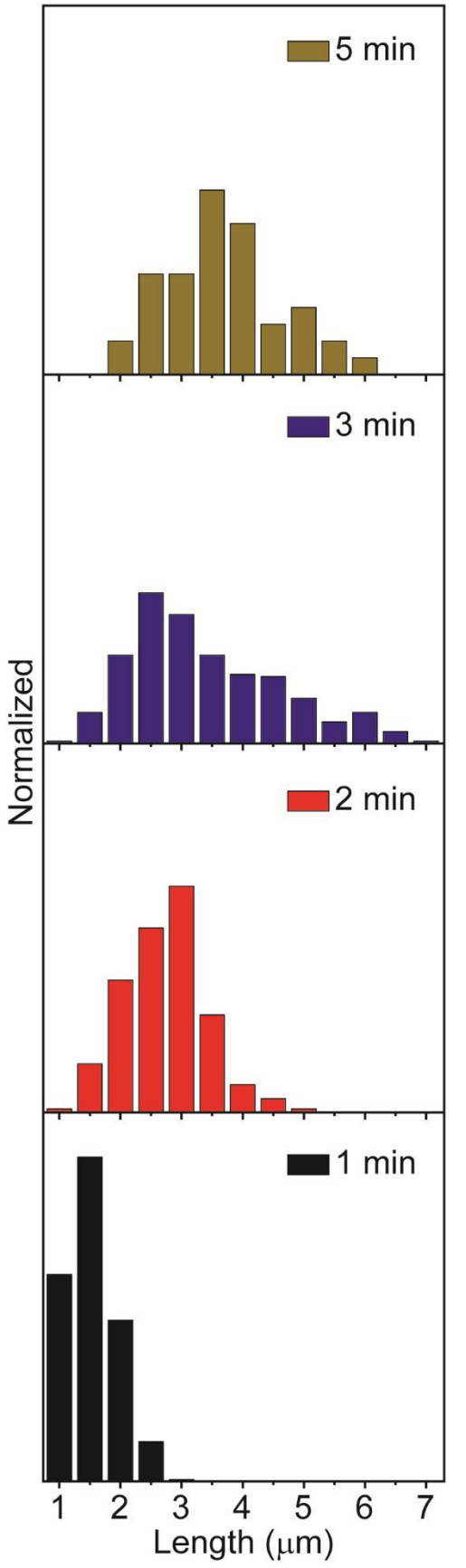

Figure S3: Distribution of the $TaSe_3$ nanowire's length as a function of hold time at 400°C. As the hold is prolonged, wires grow longer and short wires deteriorate.

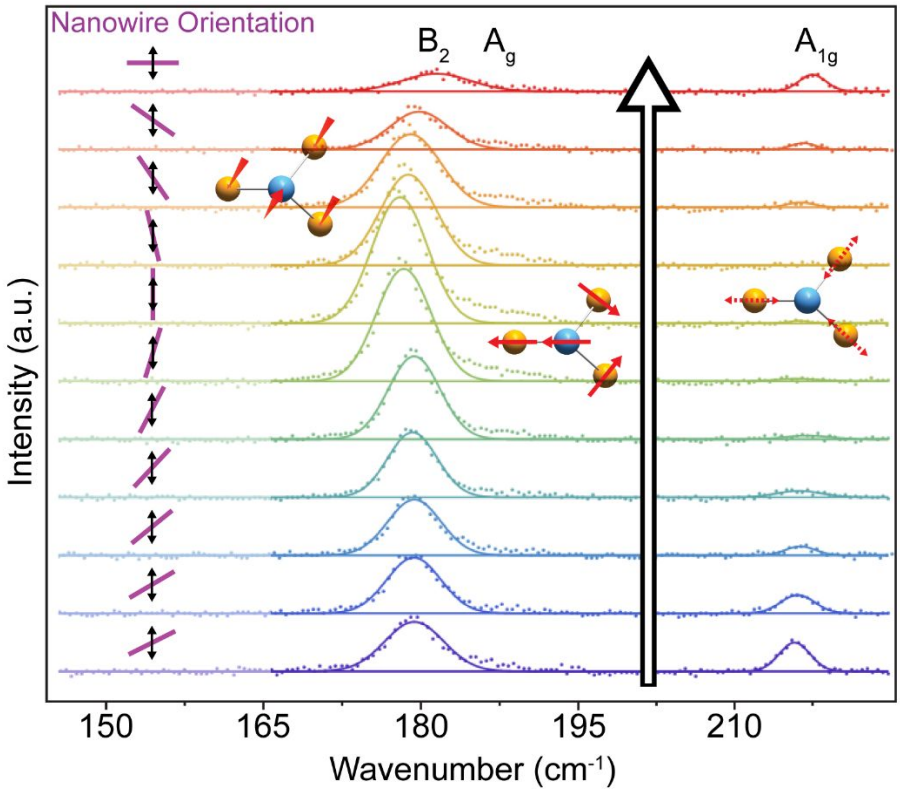

Figure S4: Dependence of the Raman spectrum of $TaSe_3$ on the angle between the plane of polarization (↕) and the nanowire (purple line). The dots represent measurements, the solid lines are Gaussian fits to the peaks. Parallel alignment shows a mode at 178-180 cm^{-1} whereas in parallel alignment and additional mode at 215-217 cm^{-1} is most pronounced. The spectra were acquired from bottom to top (vertical arrow); slight degradation of the nanowire over time is visible in the high-energy shoulder of the 178-180 cm^{-1} peak and reduced overall signal.

Computational modeling reveals near 178 cm^{-1} two modes, one associated with longitudinal wagging motion of the Ta atoms relative to the Se trimers (B2) and one associated with a scissoring of two selenium atoms about the third and the tantalum atom (Ag). At about 216 cm^{-1} three modes are found that represent symmetric and antisymmetric stretching motion of the Se trimer about the Ta atom (A1g). The direction of displacement of the atoms in these modes matches the polarization dependence of the Raman signal.

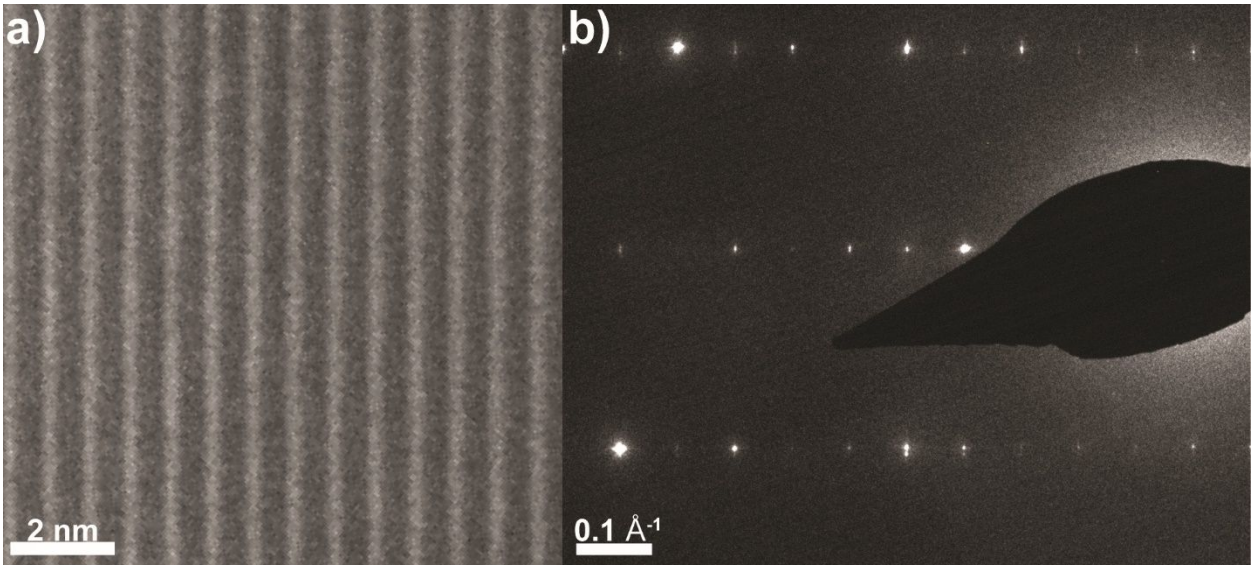

Figure S5: Representative scanning transmission electron microscopy (STEM) image and diffraction pattern of a $TaSe_3$ nanowire.

References:

1. Beyne, S.; Croes, K.; De Wolf, I.; Tokei, Z., 1/f noise measurements for faster evaluation of electromigration in advanced microelectronics interconnections. *Journal of Applied Physics* **2016,** 119, (18), 184302.
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