Supplementary Information

Atomistically Observing Real-Space Structure of Compositon Modulated $(Nb_{0.94}V_{0.06})_{10}$ $(Si_xGe_{1-x})_7$ Nanowires with Ultralow Resistivity

Sunghun Lee,^{a‡} Juneho In,^a Si-in Kim,^a Yun Chang Park,^b Hyunju Kim,^a Hana Yoon,^a Jinhee Kim,^c Sungyul Lee^{*d} and Bongsoo Kim^{*a}

^aDepartment of Chemistry, KAIST, Daejeon, 305-701, Korea E-mail: <u>bongsoo@kaist.ac.kr</u>

^cMeasurement and Analysis Team, NNFC, Daejeon, 305-806, Korea

^dCenter for Electricity and Magnetism, KRISS, Daejeon, 305-340, Korea

^eDepartment of Applied Chemistry, Kyung Hee University, Kyungki, 446-701, Korea E-mail: sylee@khu.ac.kr

^{*}Present status: Semiconductor Device Laboratory, Samsung Advanced Institute of Technology, Gyeonggi-do, 446-712, Korea **Table S1.** Si and Ge atoms inserted in Ge atom columns of $Nb_{10}Ge_7$ unit cell for STEM simulation. (The coordinates of Ge atom columns are provided at the following site: icsd.kisti.re.kr.)

Coordinates	(0.25000, 0.60850, 0.00000)	(0.50000, 0.00000, 0.00000)
Nb ₁₀ Ge ₇	# of Ge : 6	# of Ge : 1
$Nb_{10}(Si_{0.5}Ge_{0.5})_7$	# of Ge : 3.5	# of Si : 2
	# of Si : 1.5	



Fig. S1 Representative HRTEM images from the region I, II, and III of the as-synthesized $(Nb_{0.94}V_{0.06})_{10}(Si_xGe_{1-x})_7$ nanowire showing the clear lattice fringes along the nanowire axis.



Fig. S2 TEM results of Nb₁₀(Si_{*x*}Ge_{1-*x*})₇ ($0 \le x \le 0.5$) NWs obtained on sapphire substrates at the substrate temperatures of 870-900 °C. First column: low resolution TEM images, as-synthesized NWs have the lengths of tens of micrometers and the diameters of 10-30 nm as well as a clear surface. Second column: HRTEM images of the NWs show the clear lattice fringes aligned along radial and axial directions. Third column: STEM-EDS spectra of the NWs exhibit that the relative composition ratio of Si (red arrow) to Ge (blue arrow) increases in the NW as the substrate temperature increases, which is consistent with fourth column of Fig. 2.



Fig. S3 Representative X-ray diffraction (XRD) pattern of $(Nb_{0.94}V_{0.06})_{10}(Si_xGe_{1-x})_7$ NW ensembles synthesized on a vanadium foil. Most of the peaks are indexed to hexagonal Nb₁₀Ge₇ crystal phase (JCPDS card no. 72-1028). Red and blue arrows indicate the peaks from vanadium foil (JCPDS card no. 22-1058) and V₃Ge (JCPDS card no. 65-6518), respectively.