

Electronic supplementary information

**Power generation from the $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$ -based single thermoelectric
element with Au diffusion barrier**

Raju Chetty^a, Yuta Kikuchi^a, Yohan Bouyrie^a, Priyanka Jood^a, Atsushi Yamamoto^a,

Koichiro Suekuni^b, and Michihiro Ohta^{a*}

*^a Research Institute for Energy Conservation, National Institute of Advanced Industrial Science
and Technology (AIST), Tsukuba, Ibaraki 305-8568, Japan*

*^b Department of Applied Science for Electronics and Materials, Interdisciplinary Graduate
School of Engineering Sciences, Kyushu University, Kasuga, Fukuoka 816-8580, Japan*

*Corresponding Author: Michihiro Ohta

Email: ohta.michihiro@aist.go.jp

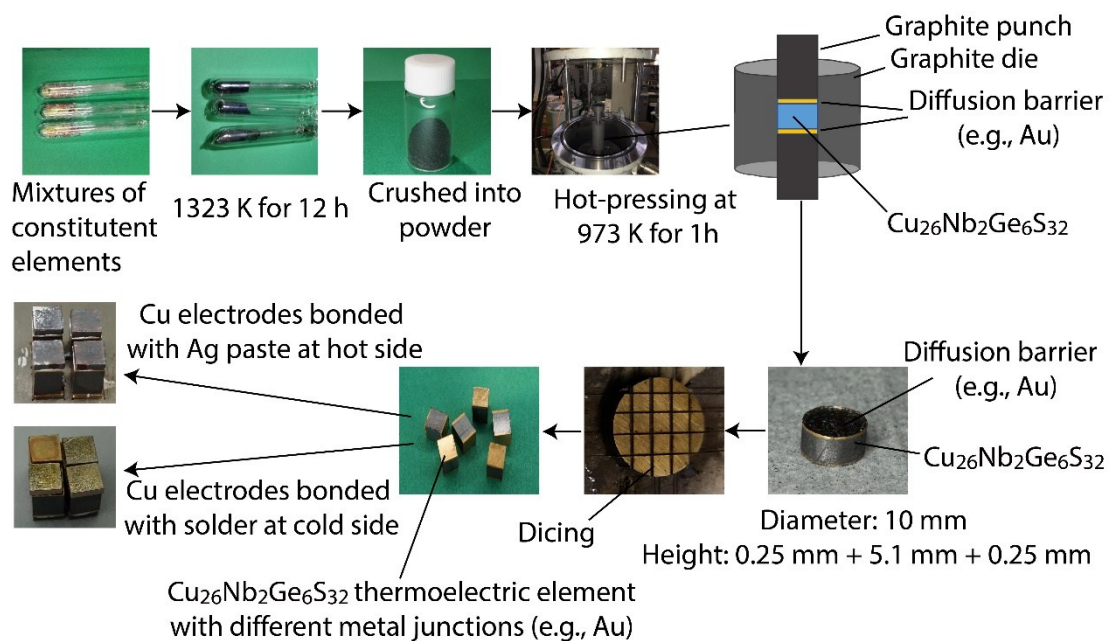


Figure S1

Preparation of Cu₂₆Nb₂Ge₆S₃₂ thermoelectric elements with different metal junctions.

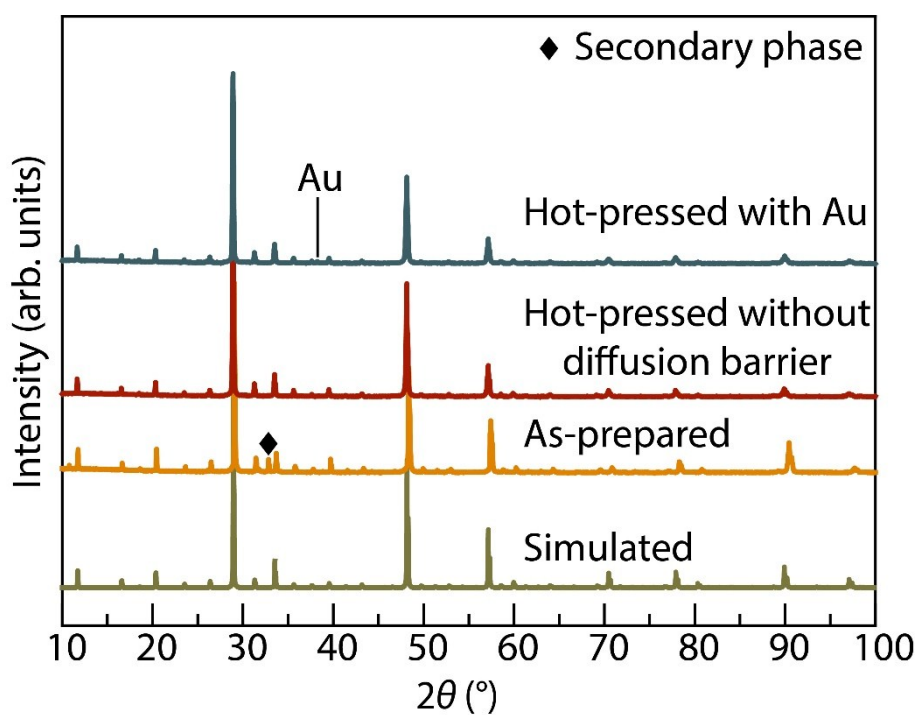


Figure S2

Powder X-ray diffraction patterns of simulated, as-prepared $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$, hot-pressed $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$ without diffusion barrier, and hot-pressed $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$ with Au over the range of 10° – 100° .

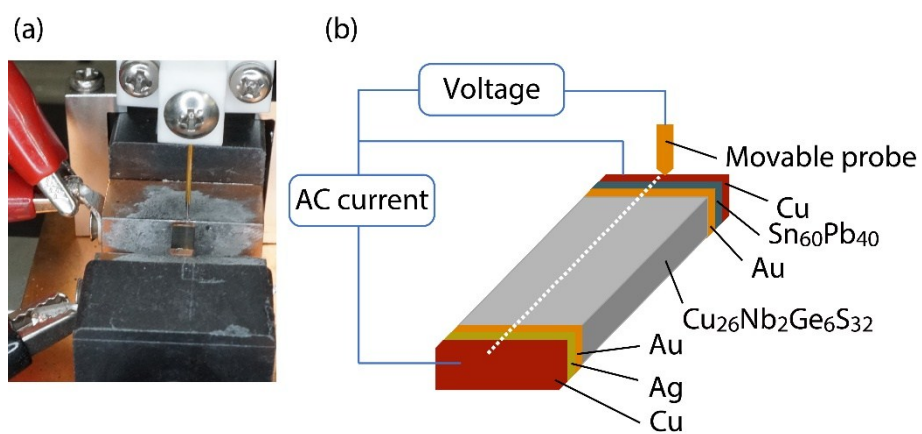


Figure S3

(a) Photograph of sample mounted and (b) a schematic diagram for the electrical resistance (R) measurement setup.

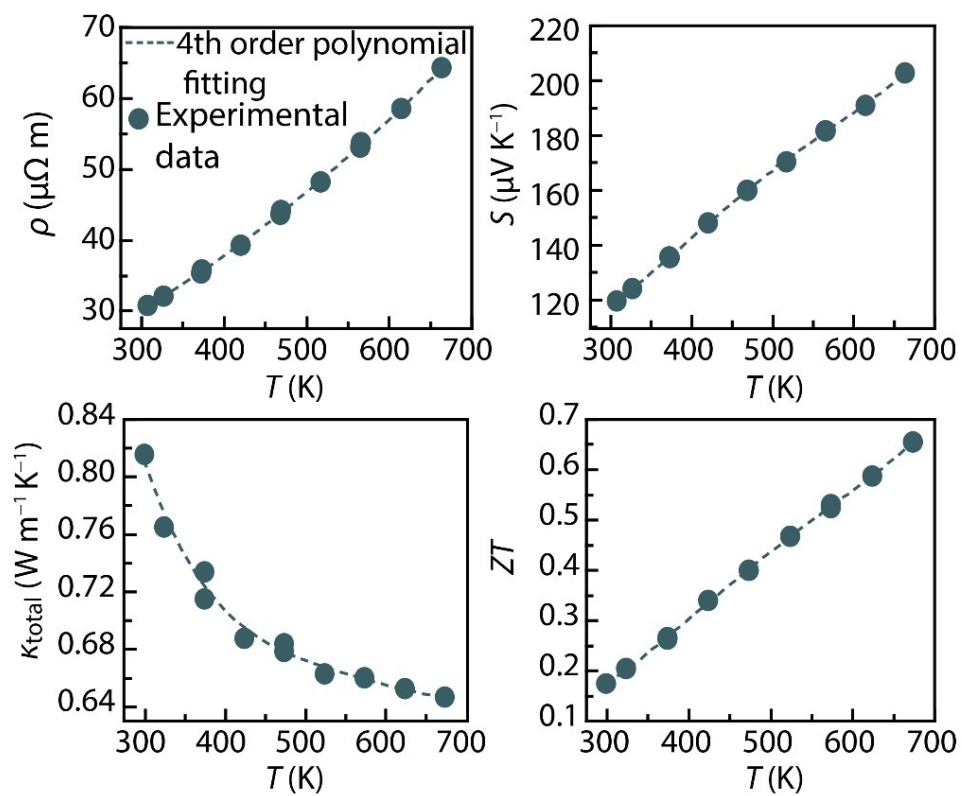


Figure S4

Fourth order polynomial fittings of temperature dependent electrical resistivity (ρ), Seebeck coefficient (S), total thermal conductivity (κ_{total}) and thermoelectric figure of merit (ZT).

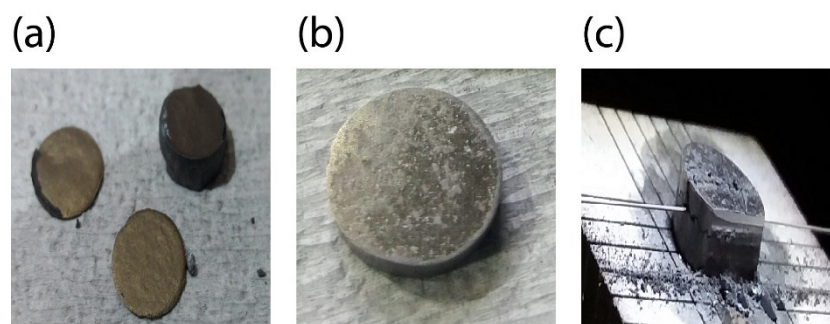


Figure S5

(a) Hot-pressed sample of Ti foil/ $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$ /Ti foil after hot pressing at 973 K. Ti foil was peeled off. (b) hot-pressed sample of Ti powder/ $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$ /Ti powder after hot pressing at 973 K. (c) The Ti layer peeled off during the dicing.

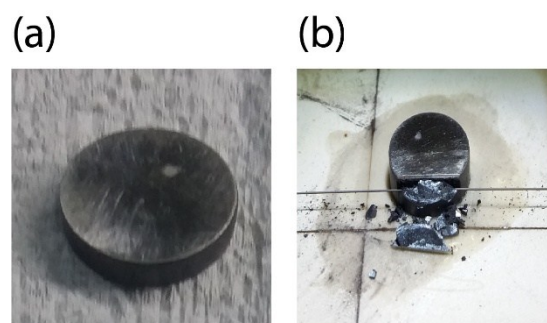


Figure S6

(a) Hot-pressed sample of Pt foil/ $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$ /Pt foil after hot pressing at 973 K. (b) The Pt layer was peeled off during the dicing.

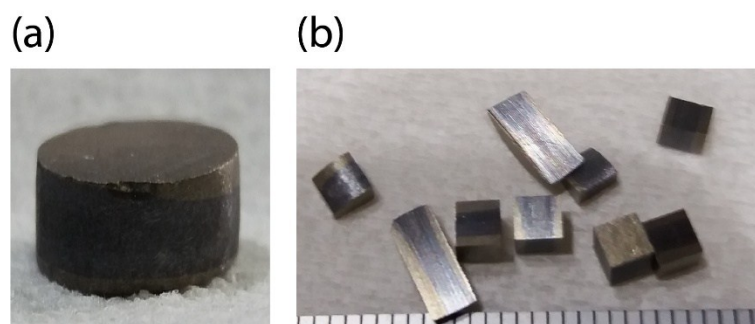


Figure S7

(a) Hot-pressed sample of Ni powder/Cu₂₆Nb₂Ge₆S₃₂/Ni powder sample after hot pressing at 923

K. (b) Hot pressed elements of Ni powder/Cu₂₆Nb₂Ge₆S₃₂/Ni powder after dicing.

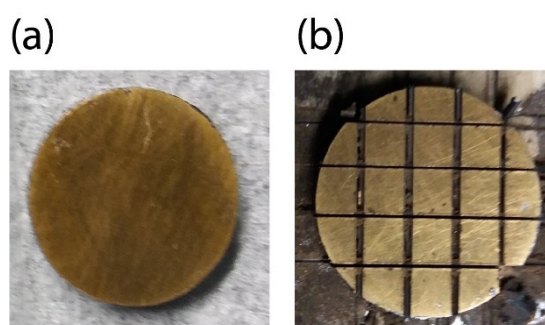


Figure S8

(a) Hot-pressed sample of Au foil/Cu₂₆Nb₂Ge₆S₃₂/Au foil after hot pressing at 973 K.(b) Hot

pressed elements of Au foil/Cu₂₆Nb₂Ge₆S₃₂/Au foil after the dicing.

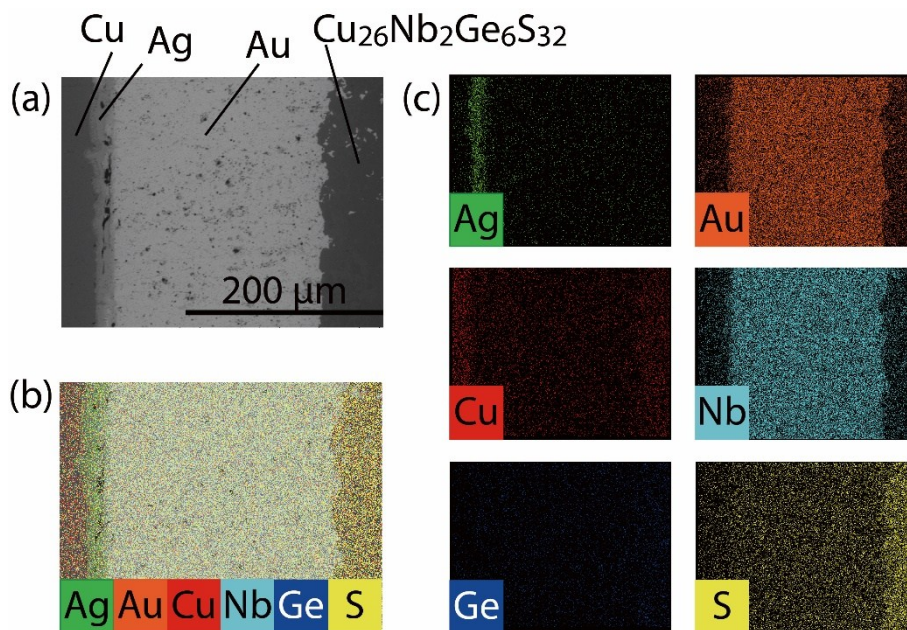


Figure S9

(a) Scanning electron microscopy backscattered electron (SEM-BSE) image of Cu/Ag/Au/ $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$ interface in hot side, and (c) and (d) the corresponding X-ray maps of Cu, Ag, Au and $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$. Note that the energy of Nb $L\alpha_1 = 2.169$ keV is close to the energy of Au $M\alpha_1 = 2.123$ keV.

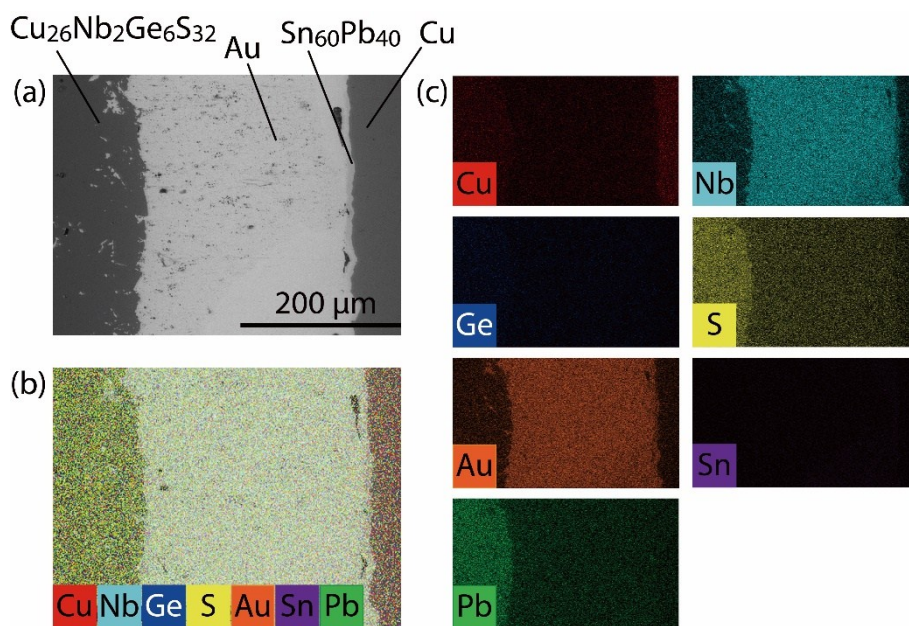


Figure S10

(a) Scanning electron microscopy backscattered electron (SEM-BSE) image of $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}/\text{Au}/\text{Sn}_{60}\text{Pb}_{40}/\text{Cu}$ interface in cold side, and (c) and (d) the corresponding X-ray maps of Au, $\text{Cu}_{26}\text{Nb}_2\text{Ge}_6\text{S}_{32}$, Sn, Pb and Cu. Note that the energy of $\text{S } K\alpha_1 = 2.309 \text{ keV}$ is close to the energy of $\text{Pb } M\alpha_1 = 2.342 \text{ keV}$.

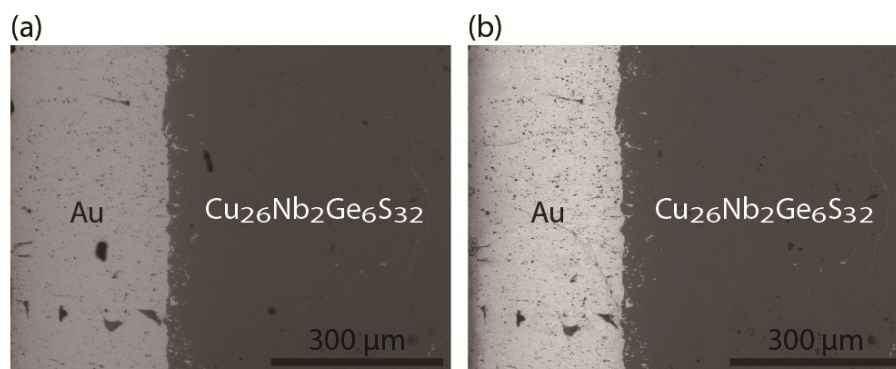


Figure S11

Scanning electron microscopy backscattered electron (SEM-BSE) image of Au/Cu₂₆Nb₂Ge₆S₃₂ interface at the hot side of thermoelectric element (a) before and (b) after the temperature gradient treatment, respectively.