High electron mobility and transverse negative magnetoresistance in van der Waals material Nb_2GeTe_4

Xue Han,[a] Zhongnan Guo,[*a] Long Chen,[b,c] Cheng Cao,[b,c] Gang Wang, [b,d,e] and Wenxia Yuan[*a]

[a] *Department of Chemistry, School of Chemistry and Biological Engineering, University of Science and Technology Beijing, Beijing 100083, China*

[b] *Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Sciences, Beijing, 100190, China*

[c] *University of Chinese Academy of Sciences, Beijing 100049, China*

[d] *School of Physical Sciences, University of Chinese Academy of Sciences, Beijing 100049, China*

[e] *Songshan Lake Materials Laboratory, Dongguan, Guangdong 523808, China*

*Authors to whom correspondence should be addressed: guozhongn@ustb.edu.cn and wxyuanwz@163.com

Table S1. Crystal data and structure refinement for Nb_2GeTe_4 at 293 K.

Empirical formula	Nb_2GeTe_4
Wavelength	0.71073 Å
Crystal system	monoclinic
Space group	$P2_1/n$
	a = 6.4601(8) Å, α = 90°
Unit cell dimensions	b = 7.9259(10) Å, β = 97.843(4)°
	c = 14.2127(17) Å, γ = 90°
Volume	720.91(15) $Å^3$
Z	1
θ range for data collection	2.893 to 28.299°
Index ranges	$-6\leq h\leq 8$, $-10\leq k\leq 10$, $-18\leq l\leq 18$
Reflections collected	7635
Independent reflections	1742 [R_{int} = 0.0513]
Completeness to θ = 25.242°	96.8%
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	1742 / 0 / 64
Goodness-of-fit	1.180
Final R indices [I > 2σ(I)]	R_{obs} = 0.1242, wR_{obs} = 0.3311
R indices [all data]	R_{all} = 0.1251, wR_{all} = 0.3318

$R = \Sigma||F_o|-|F_c|| / \Sigma|F_o|$, $wR = \{\Sigma[w(|F_o|^2 - |F_c|^2)^2] / \Sigma[w(|F_o|^4)]\}^{1/2}$ and $w=1/[\sigma^2(Fo^2)+(0.1846P)^2+170.5381P]$ where $P=(Fo^2+2Fc^2)/3$

Table S2. Atomic coordinates (×10^4) and equivalent isotropic displacement parameters ($Å^2$×10^3) for Nb_2GeTe_4 at 293 K with estimated standard deviations in parentheses.

Label	x	y	z	Occupancy	U_{eq}*
Te(1)	2453(3)	7395(2)	1162(2)	1	4(1)
Te(2)	-1751(3)	10123(2)	3838(2)	1	3(1)
Te(3)	-2556(2)	10126(2)	1153(2)	1	3(1)
Te(4)	1725(2)	12426(2)	1154(2)	1	3(1)
Nb(1)	1060(3)	9656(3)	2494(2)	1	2(1)
Nb(2)	6066(3)	7858(3)	2499(2)	1	1(1)
Ge(1)	12(4)	6263(3)	2510(2)	1	3(1)

*U_{eq} is defined as one third of the trace of the orthogonalized U_{ij} tensor.

Table S3. Anisotropic displacement parameters ($Å^2$×10^3) for Nb_2GeTe_4 at 293 K with estimated standard deviations in parentheses.

Label	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Te(1)	4(1)	2(1)	6(1)	-1(1)	2(1)	0(1)
Te(2)	3(1)	2(1)	5(1)	-3(1)	1(1)	0(1)
Te(3)	2(1)	2(1)	6(1)	-2(1)	2(1)	1(1)
Te(4)	2(1)	2(1)	6(1)	1(1)	3(1)	0(1)
Nb(1)	0(1)	-1(1)	8(2)	0(1)	3(1)	-1(1)
Nb(2)	0(1)	-1(1)	5(2)	0(1)	2(1)	0(1)
Ge(1)	-1(2)	0(2)	10(2)	0(1)	2(1)	0(1)

The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2a^{*2}U_{11} + ... + 2hka^*b^*U_{12}]$.

Table S4. The details of Hall resistivity data plotted in Figure 3**.**

T(K)	R_H (cm^3C^{-1})	ρ_{xx} ($\Omega\cdot cm$)	μ ($cm^2V^{-1}s^{-1}$)	n ($\times 10^{18}cm^{-3}$)
5	-2.37	2.7092	0.88	2.64
10	-1.96	0.8318	2.36	3.19
50	-1.69	0.0278	60.98	3.69
100	-1.51	0.0049	307.73	4.13
150	-1.31	0.0028	476.23	4.77
200	-1.15	0.0022	518.28	5.45
300	-0.88	0.0021	424.37	7.11

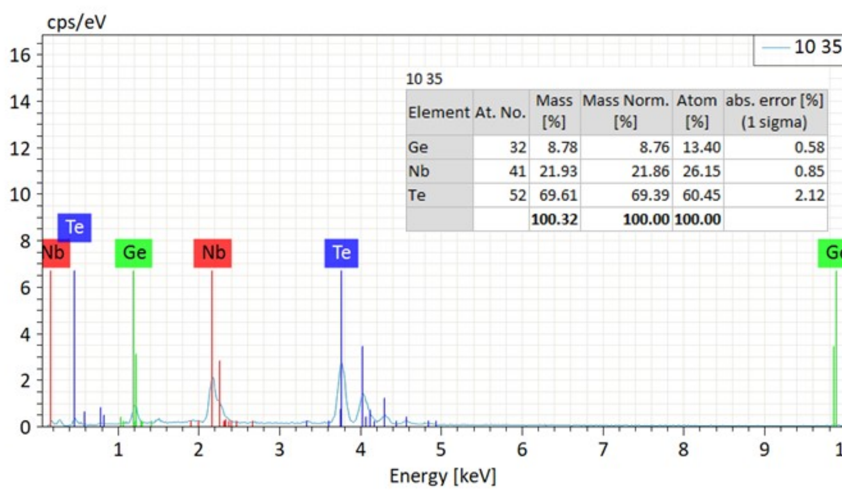

Figure S1. EDS measurement indicates the atomic ratios of Nb, Ge and Te elements.

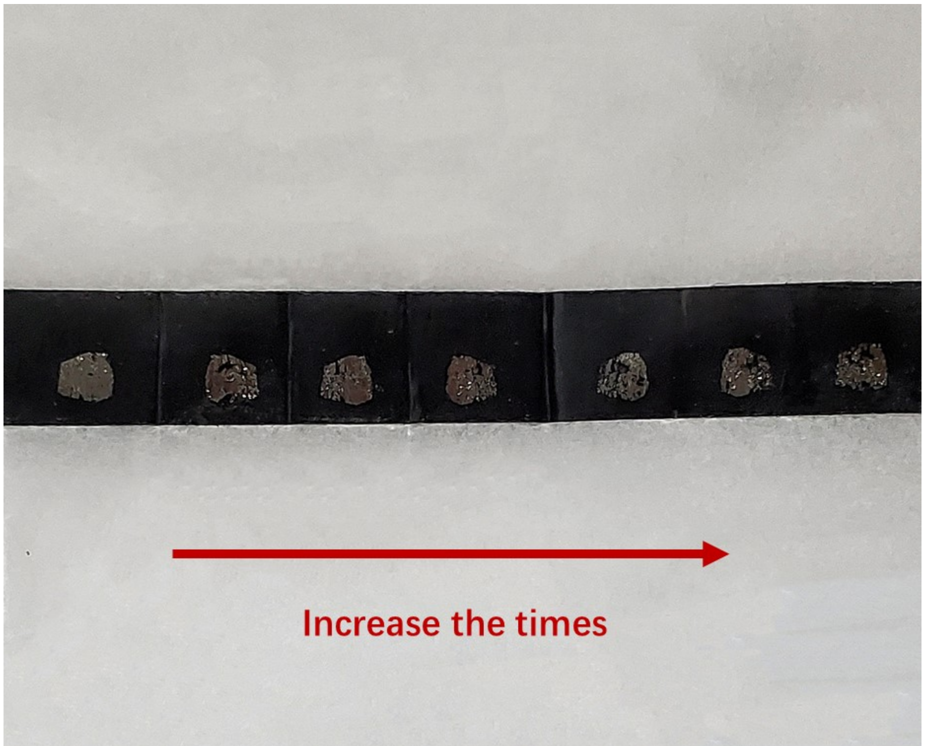

Figure S2. The photo of Nb_2GeTe_4 thin flakes, which can be easily obtained by mechanical exfoliation using Scotch-tape method.

.

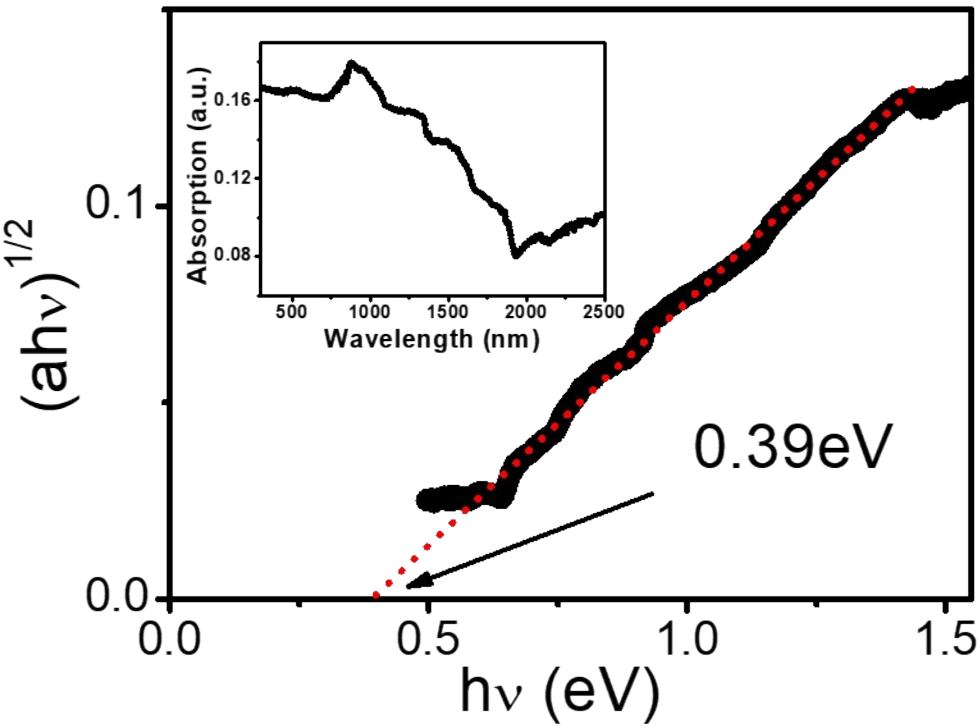

Figure S3. UV-vis-NIR absorption spectra (inset) and the plots of $(ahv)^{1/2}$ versus photo energy of Nb_2GeTe_4