Supplementary Information

Exploring the Interplay between Structure and Electronic Behavior across Pressure-Induced Isostructural and Structural Transitions in Weyl-type Semimetal NbAs

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Figures

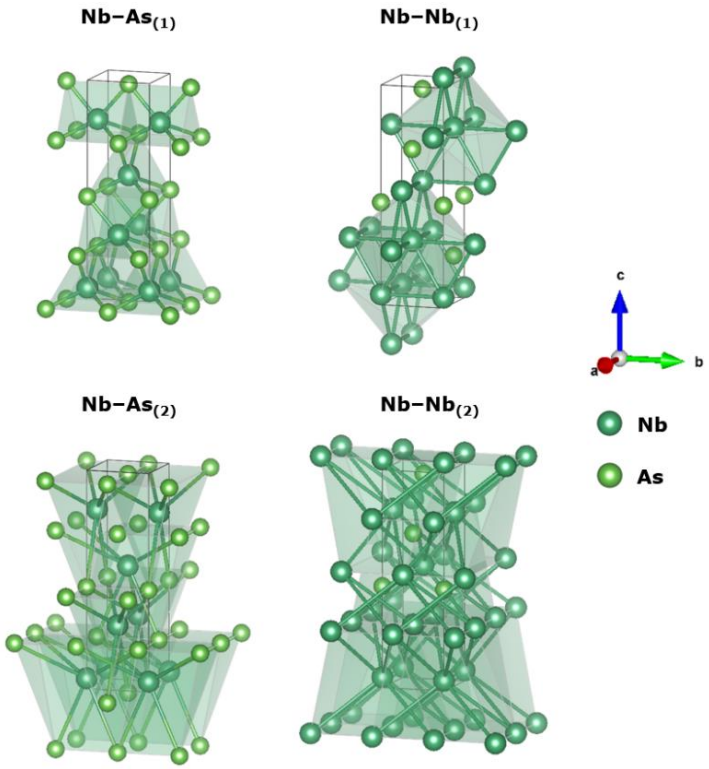

Figure S1. Sketch of the single scattering paths [Nb–As$_{(1)}$, Nb–Nb$_{(1)}$, Nb–As$_{(2)}$, and Nb–Nb$_{(2)}$] employed to model EXAFS fitting in Weyl semimetal NbAs.

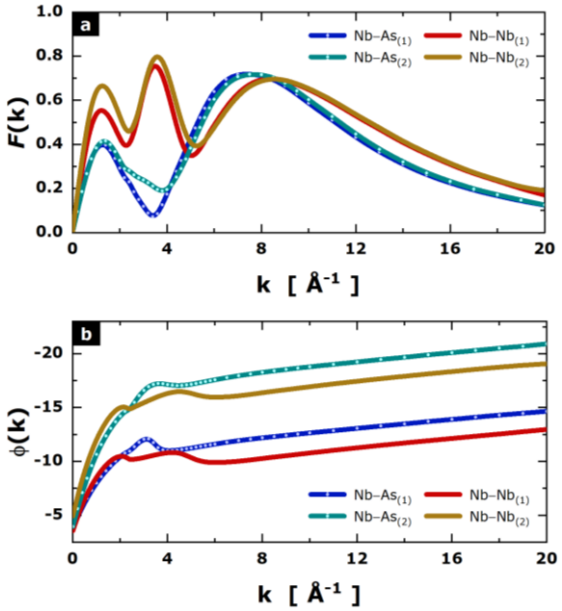

Figure S2. The backscattering amplitude [$F(k)$] (a) and phase [$\phi(k)$] (b) for single scattering paths [Nb–As$_{(1)}$, Nb–Nb$_{(1)}$, Nb–As$_{(2)}$, and Nb–Nb$_{(2)}$] calculated using FEFF method [39].

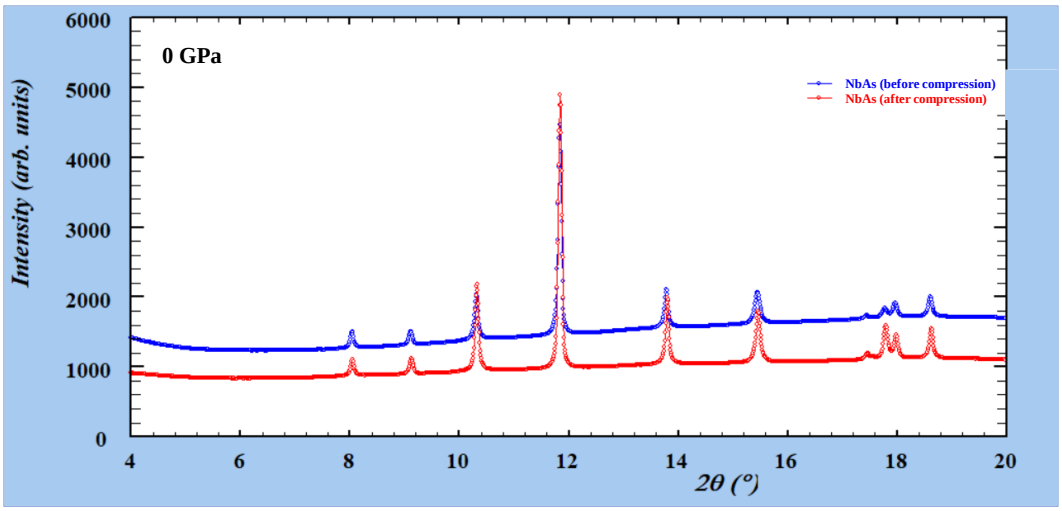

Figure S3. Comparison between SXRD patterns collected at ~0 GPa before and after the compression run.

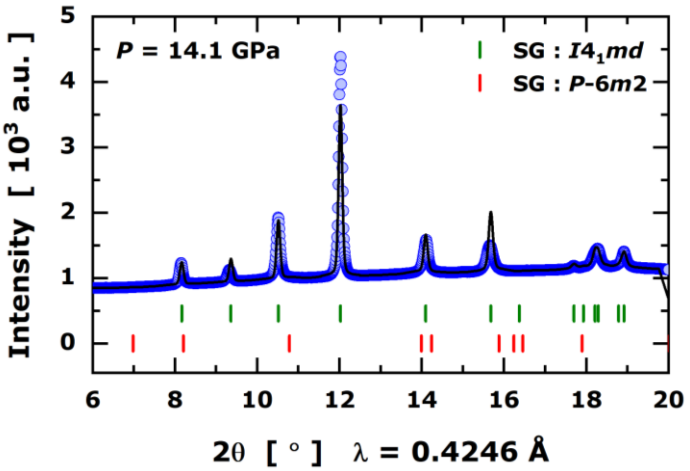

Figure S4. Integrated diffraction pattern of NbAs at ~14.1 GPa (blue open circles) and the Rietveld refinement (black line), and the green/red bars represent the expected Bragg reflections (tetragonal/hexagonal phases).

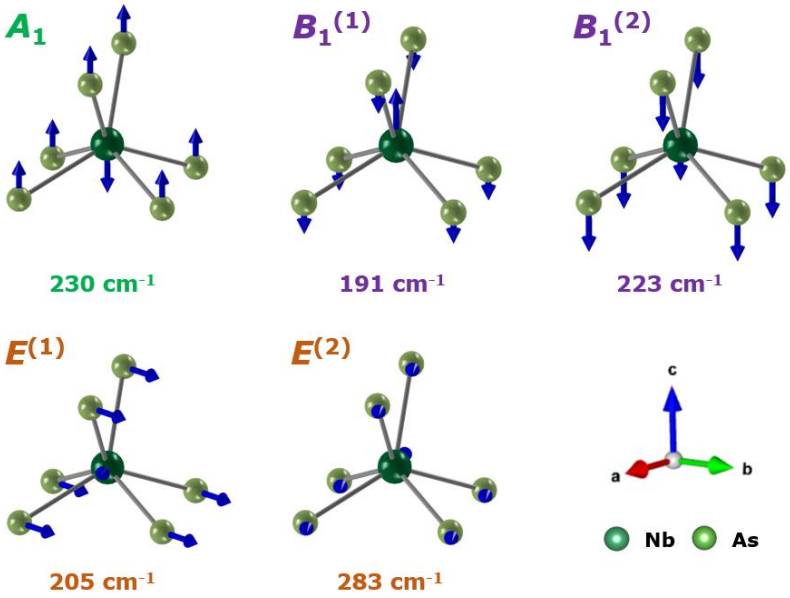

Figure S5. The vibrational patterns for five vibrational modes ($A_1 \oplus 2B_1 \oplus 2E$) in the tetragonal structure of the Weyl semimetal NbAs were determined, with the calculated wavenumbers obtained using the GF-matrix method (LDC, lattice dynamics calculations) [42]. Blue arrows represent the atomic displacement patterns.

Tables

Table S1. Structural parameters theoretically predicted for different phases of Weyl semimetal NbAs (SG: $I4_1md$, $P\bar{6}m2$, $P2_1/c$, and $Pm\bar{3}m$) under ambient conditions, as reported in Ref [26].

	$I4_1md$	$P\bar{6}m2$	$P2_1/c$	$Pm\bar{3}m$
a (Å)	3.4726	3.4253	6.0999	3.2192
b (Å)	3.4726	3.4253	4.933	3.2192
c (Å)	11.7569	3.4863	6.22	3.2192
α (°)	90	90	90	90
β (°)	90	90	132.0642	90
γ (°)	90	120	90	90
Nb (x,y,z)	(0.0, 0.0, 0.04798)	(0.33333, 0.66667, 0.0)	(−0.67755, 0.64216, −0.30150)	(0.5, 0.5, 0.5)
As (x,y,z)	(0.5, 0.5, 0.96614)	(0.0, 0.0, 0.5)	(−0.20693, 0.65032, −0.27372)	(0.0, 0.0, 0.0)

Table S2. Pressure dependence of the structural parameters (a, c, and V) extracted from Rietveld refinements of the high-pressure XRD data of NbAs. Uncertainties correspond to those obtained from the refinements.

P ± 0.1 (GPa)	a (Å)	δa (Å)	c (Å)	δc (Å)	V (Å^3)	δV (Å^3)
0	3.45368	9.3×10^{-4}	11.68451	0.0041	139.372	0.072
0.22	3.45024	8.1×10^{-4}	11.65948	0.00362	138.796	0.063
0.39	3.44878	6.6×10^{-4}	11.65876	0.00288	138.67	0.051
0.9	3.44741	6.7×10^{-4}	11.64802	0.00295	138.432	0.052
1.61	3.44538	6.9×10^{-4}	11.63355	0.00304	138.098	0.053
2.35	3.4426	7.0×10^{-4}	11.6162	0.00309	137.669	0.054
3.01	3.44038	7.5×10^{-4}	11.60257	0.00331	137.331	0.058
3.86	3.43574	6.6×10^{-4}	11.58029	0.00286	136.697	0.05
4.41	3.43375	6.8×10^{-4}	11.56936	0.00293	136.41	0.051
5.01	3.43062	6.9×10^{-4}	11.55303	0.003	135.969	0.052
5.81	3.42693	7.3×10^{-4}	11.53069	0.00318	135.415	0.055
6.4	3.42489	7.5×10^{-4}	11.51636	0.00327	135.085	0.057
7.195	3.42192	8.0×10^{-4}	11.49722	0.00348	134.627	0.06
8.22	3.41732	8.2×10^{-4}	11.4794	0.00358	133.989	0.062
10.06	3.40962	9.9×10^{-4}	11.44348	0.00442	133.036	0.075
11.18	3.40706	0.00106	11.42355	0.0047	132.605	0.08
12.2	3.40414	0.001	11.39482	0.0044	132.045	0.075
13.26	3.4036	0.00103	11.38943	0.00454	131.941	0.077
14.1	3.40274	0.00115	11.376	0.00501	131.719	0.085

Table S3. Factor-group analysis for the tetragonal and hexagonal crystal structures of Weyl semimetal NbAs [60]. Abbreviations: *T*, total; *A*, acoustic; *IR*, infrared; *R*, Raman.

Atom	Wyckoff site	Symmetry	Irreducible representation
Tetragonal: $I4_1md$ (factor-group: C_{4v})			
Nb	4a	$2mm$ (C_{2v}^{v})	$A_1 \oplus B_1 \oplus 2E$
As	4a	$2mm$ (C_{2v}^{v})	$A_1 \oplus B_1 \oplus 2E$
Γ_T	$2A_1 \oplus 2B_1 \oplus 4E$	Γ_{IR}	$A_1 \oplus 3E$
Γ_A	$A_1 \oplus E$	Γ_R	$A_1 \oplus 2B_1 \oplus 3E$
Hexagonal: $P\bar{6}m2$ (factor-group: D_{3h})			
Nb	1c	$\bar{6}m2$ (D_{3h})	$A''_2 \oplus E'$
As	1b	$\bar{6}m2$ (D_{3h})	$A''_2 \oplus E'$
Γ_T	$2A''_2 \oplus 2E'$	Γ_{IR}	$A''_2 \oplus E'$
Γ_A	$A''_2 \oplus E'$	Γ_R	E'

Table S4. List of experimental and calculated vibrational modes under ambient conditions for tetragonal NbAs. To model the short-range bonding [42], three force constants were used as follows: Nb–As (k_1 ~ 0.867 md·Å^{-1}), As–As (f_1 ~ 0.394 md·Å^{-1}), and As–Nb–As (h_1 ~ 0.561 md-Å).

Symmetry	$\tilde{\nu}$ LDC (cm^{-1}), this work	$\tilde{\nu}$ DFT (cm^{-1}), from Ref [27]	$\tilde{\nu}$ Exp (cm^{-1}), from Ref [27]
A_1	230	274	271
B_1	191	234	234
B_1	224	256	252
E	206	150	151
E	284	260	253

Table S5. The main observations from the multiscale length structural analysis of the pressure-induced transitions in Weyl semimetal NbAs, using XRD and XAS data, obtained in this work.

Scale	Property	Parameter	Lifshitz (GPa)	Comment	Tetra-to-Hexa (GPa)	Comment
Bulk **(XRD)**	*Structural*	Unit-cell volume	~12	Slight change in compressibility	23–26	Predicted in Ref [26]
Medium **(XANES)**	*Atomic*	XANES feature γ	-	Not visible	> 25	Calculated FDMNES
	Electronic	Edge energy shift	~12	Clear discontinuity	26–28	Progressive change
2nd nearest neighbor † **(EXAFS)**	*Atomic*	Path Nb–Nb(1)	12–15	Clear discontinuity	~25	Stagnation
	Vibrational	Variance Nb–Nb(1)	~15	Slight discontinuity	~25	Stagnation
1st nearest neighbor † **(EXAFS)**	*Atomic*	Path Nb–As(1)	~15	Slight change in compressibility	~25	Slight change
	Vibrational	Variance Nb–As(1)	-	Slight discontinuity	~25	Minimum, Progressive

† The 2nd nearest neighbor Nb–Nb(1) is at ~3.4 Å, while the 1st nearest neighbor Nb–As(1) is at ~2.6 Å.