Supplementary Information for

Pressure-Induced Charge Amorphisation in $BiNiO_3$

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Table S1. Rietveld refinement results for $BiNiO_3$ Phase-Id in space group *Pb*11 from NPD and SXRD. Lattice parameters, atomic coordination and refinement reliability R_{wp} and *GOF* are listed.

	NPD				SXPD			
P (GPa)	4.3				4.3			
T (K)	100				90			
a (Å)	5.2470(3)				5.2538(2)			
b (Å)	5.5938(3)				5.6073(2)			
c (Å)	7.6145(4)				7.6278(2)			
α (º)	90.16(1)				90.148(2)			
V (Å^3)	223.61(1)				224.71(1)			
R_{wp} (%)	2.59				6.21			
GOF	1.08				2.48			
*Pb*11 [a]	x	y	z	U_{iso} (Å^2) [b]	x	y	z	U_{iso} (Å^2) [c]
Bi1	0.726(3)	0.075(1)	0.340(3)	0.35(8)	0.726(2)	0.0711(6)	0.3368(8)	0.35
Bi2	0.239(3)	0.459(1)	0.836(3)	0.35	0.232(2)	0.4614(5)	0.848(1)	0.35
Ni1	0.251(3)	0.025(3)	0.088(2)	0.05(4)	0.24(2)	0.01(2)	0.09(1)	0.05
Ni2	0.255(3)	0.019(3)	0.584(2)	0.05	0.25(2)	0.01(2)	0.58(1)	0.05
O1	0.420(4)	0.346(3)	0.135(2)	0.01(4)	0.45(3)	0.35(2)	0.13(2)	0.01
O2	0.939(4)	0.216(3)	1.016(3)	0.01	0.88(3)	0.29(2)	1.00(2)	0.01
O3	0.082(4)	0.704(4)	0.648(2)	0.01	0.07(3)	0.60(3)	0.70(2)	0.01
O4	0.533(3)	0.795(3)	0.508(3)	0.01	0.55(3)	0.87(3)	0.58(2)	0.01
O5	0.875(2)	0.442(2)	0.332(4)	0.01	0.77(2)	0.50(2)	0.34(3)	0.01
O6	0.381(2)	0.041(2)	0.838(4)	0.01	0.42(2)	0.07(3)	0.87(3)	0.01

[a] For the *Pb*11 (No. 7) model all atom positions are 2*a*, (*x*, *y*, *z*). [b] The U_{iso} is constrained based on elements in the refinement. [c] The U_{iso} from the NPD refinement results are adapted to the SXRD refinement.

Table S2. Selected bond distances and BVS results of Bi and Ni sites from NPD Rietveld refinement results of $BiNiO_3$ Phase-Id in space group *Pb*11.

Bi1-O1	2.16(3)	Bi2-O1	2.55(3)
Bi1-O1	2.71(3)	Bi2-O1	3.61(3)
Bi1-O2	2.82(4)	Bi2-O2	2.49(3)
Bi1-O2	3.63(3)	Bi2-O2	2.19(3)
Bi1-O3	2.65(3)	Bi2-O3	2.63(3)
Bi1-O3	3.65(3)	Bi2-O3	2.15(3)
Bi1-O4	2.26(3)	Bi2-O4	2.92(3)
Bi1-O4	2.23(3)	Bi2-O4	3.49(3)
Bi1-O5	3.24(2)	Bi2-O6	3.26(2)
Bi1-O5	3.63(1)	Bi2-O6	2.46(1)
Bi1-O5	2.20(1)	Bi2-O6	2.05(2)
Bi1-O5	2.22(2)	Bi2-O6	3.34(1)
BVS	4.1	BVS	4.0

Ni1-O1	2.03(3)	Ni2-O3	2.04(3)
Ni1-O1	2.03(3)	Ni2-O3	2.11(3)
Ni1-O2	2.07(3)	Ni2-O4	2.01(3)
Ni1-O2	2.03(3)	Ni2-O4	1.99(3)
Ni1-O5	2.03(4)	Ni2-O5	2.08(4)
Ni1-O6	2.02(4)	Ni2-O6	2.05(4)
BVS	2.2	BVS	2.3

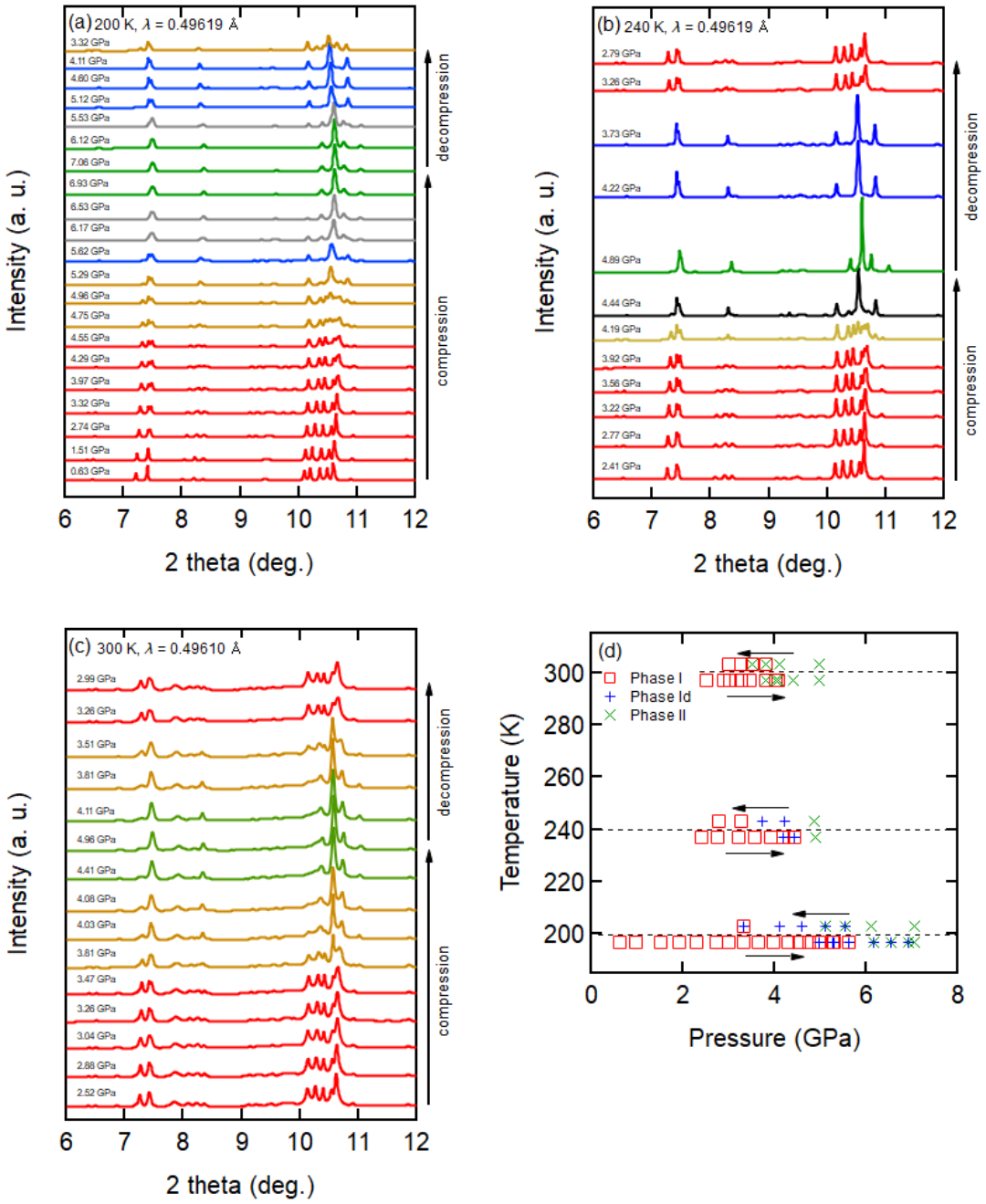

Fig. S1 Pressure-dependent synchrotron X-ray diffraction patterns of $BiNiO_3$ at (a) 200 and (b) 240 K, and (c) 300 K on compression and decompression, showing the phase transition from Phases-I to Id to II and *vice versa*. Red, blue and green lines indicate Phase-I, Id and II, respectively. Brown and grey lines denote the coexistence of two phases. Black line indicates the coexistence of three phases. (d) The pressure and temperature conditions of phase transitions and hysteresis are represented.

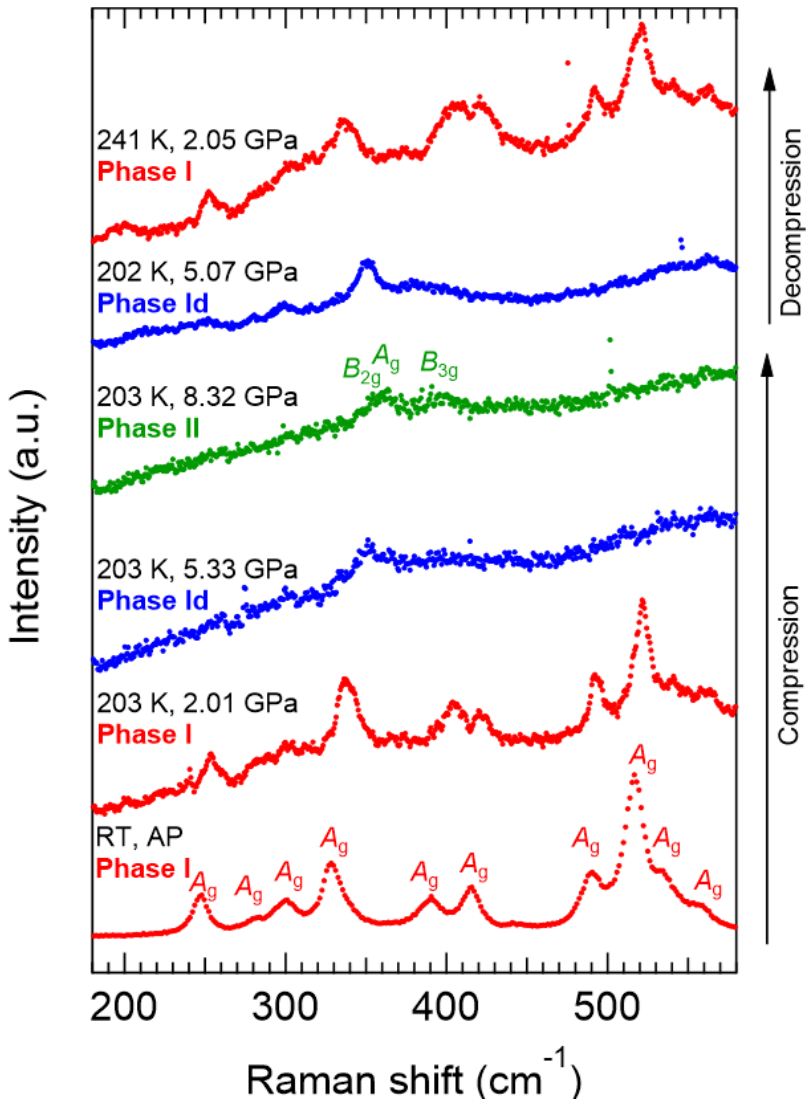

Fig. S2 Raman spectra of $BiNiO_3$ Phases-I, Id and II measured at high-pressure low-temperature conditions.

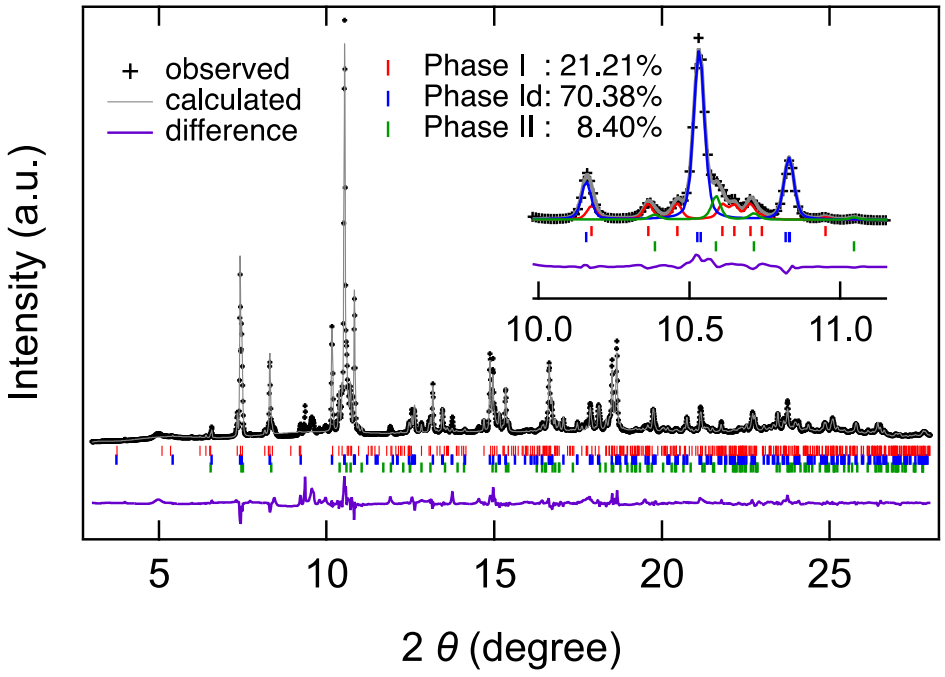

Fig. S3 Rietveld refinement result of $BiNiO_3$ at triple point (240 K and 4.44 GPa).

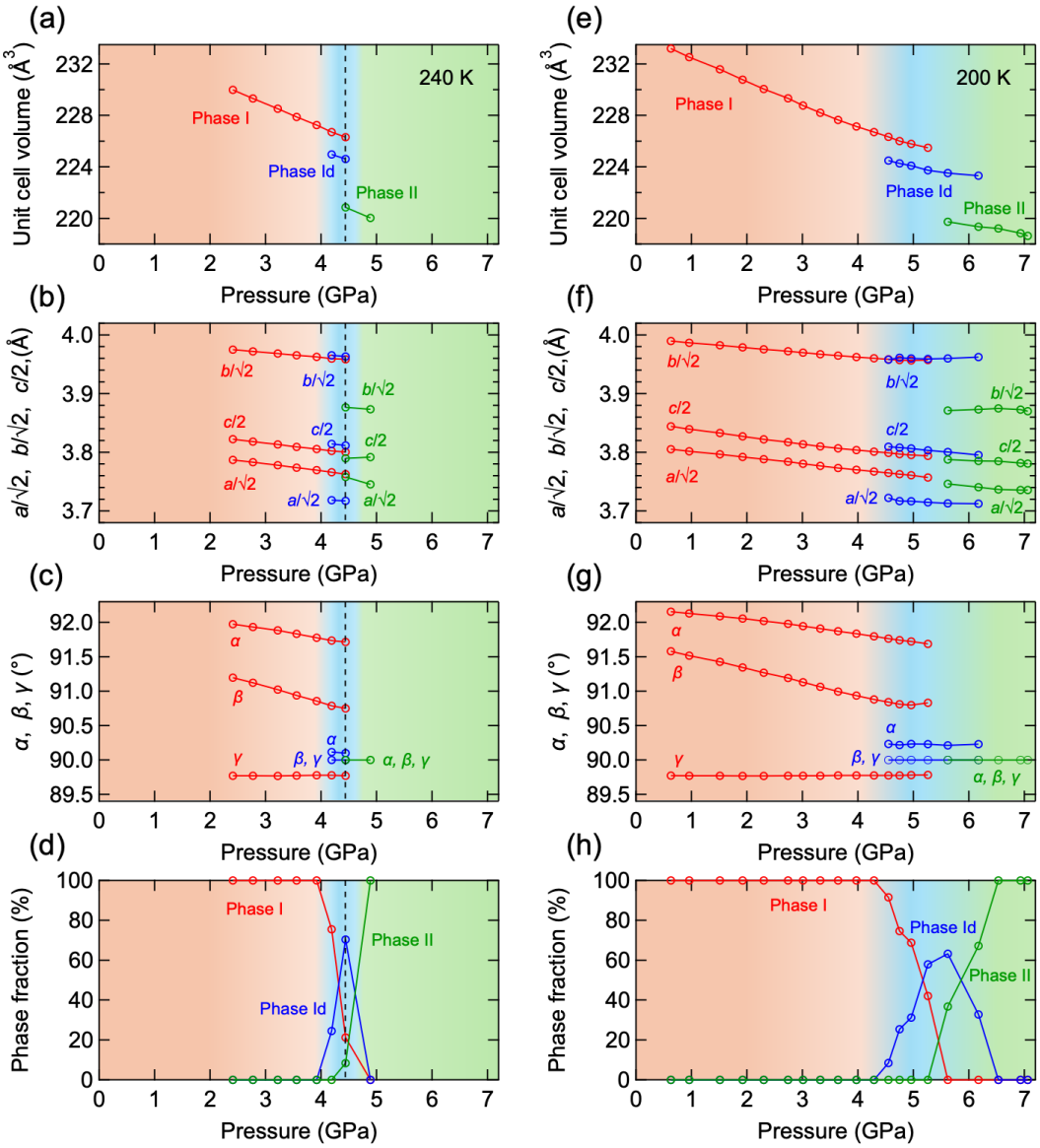

Fig. S4 Pressure dependence of unit cell volume (a, e), lattice constants (b, c, f, g) and phase fraction (d, h) at 240 K (a-d) and 200 K (e-h) obtained from the Rietveld refinements of SXRD data.

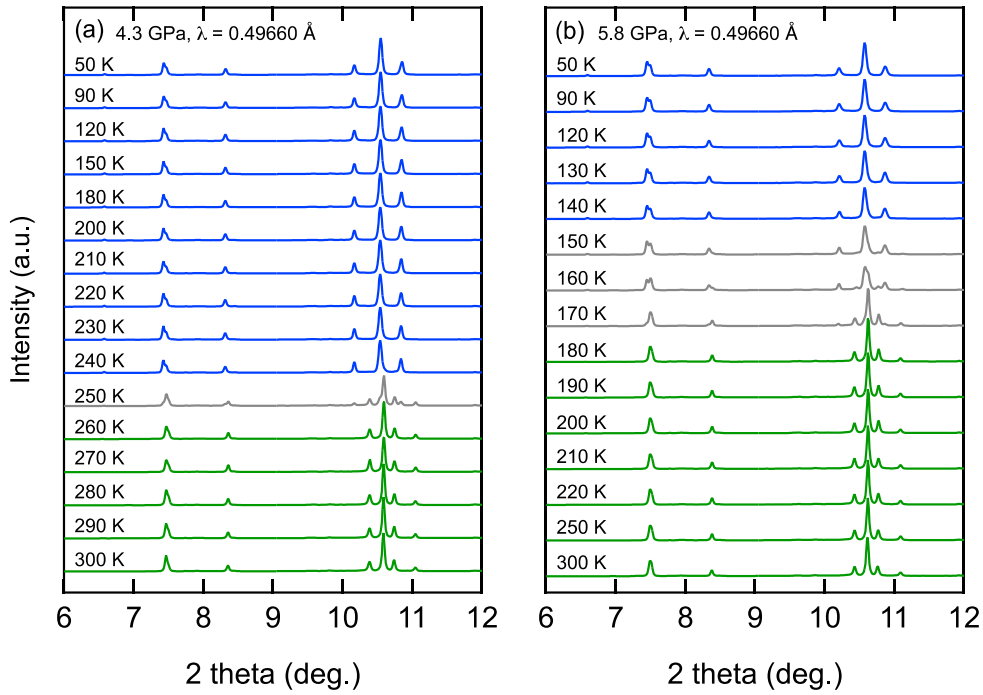

Fig. S5 Temperature-dependent synchrotron X-ray diffraction patterns of $BiNiO_3$ at (a) 4.3 and (b) 5.8 GPa on cooling. Green, blue and grey lines indicate Phase-II, Id and the coexistence of both phases, respectively.