Supporting Information

Structure of $Bi_2Rh_3Se_2$ above and below charge density wave transition determined by Bi $L\alpha$ and $L\gamma$ X-ray fluorescence holography

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The XRD pattern of $Bi_2Rh_3Se_2$ is shown in Figure S1, together with the calculated pattern based on Le Bail analysis with the large β-cell structure. The atomic arrangements which are predicted to be observed as reconstructed atomic image at z = 0 Å in the small β-cell, large β-cell and supercell structures are shown in Figure S2. Table S1 – S3 provides the atomic coordinates employed for the model structures of $Bi_2Rh_3Se_2$ (small β-cell, large β-cell and supercell structures). These atomic coordinates are basis for experimental determination of crystal structures using X-ray fluorescence holograms.

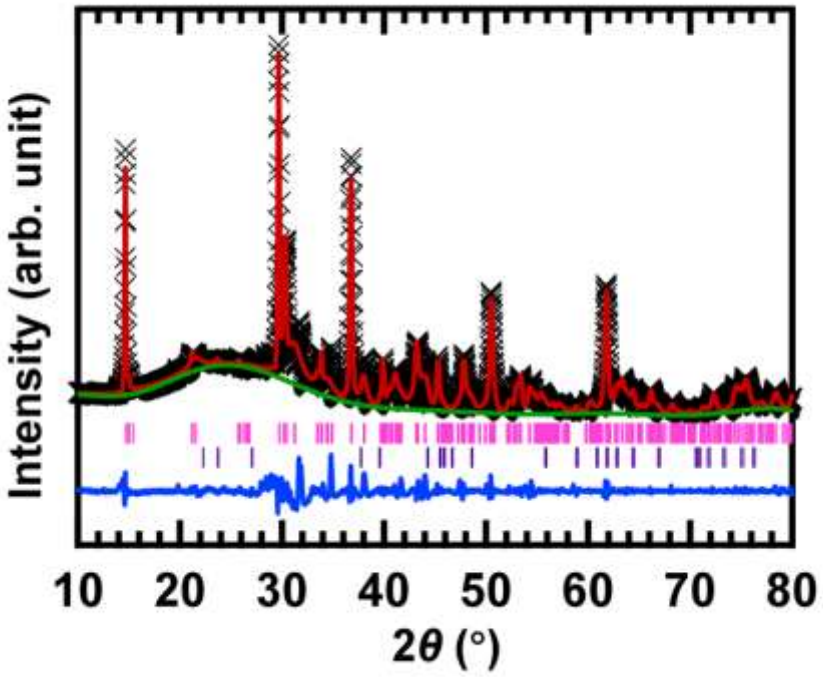

Figure S1. Powder XRD pattern of $Bi_2Rh_3Se_2$. The black symbols (x) and red lines refer to the experimental and calculated patterns, and pink and purple sticks refer to the positions of Bragg reflections due to $Bi_2Rh_3Se_2$ and Bi, respectively. The blue lines refer to the difference between the experimental and calculated patterns. The calculation was made by Le Bail analysis with large β-cell structure (see text) under the space group of *C*2/*m* (No. 9).

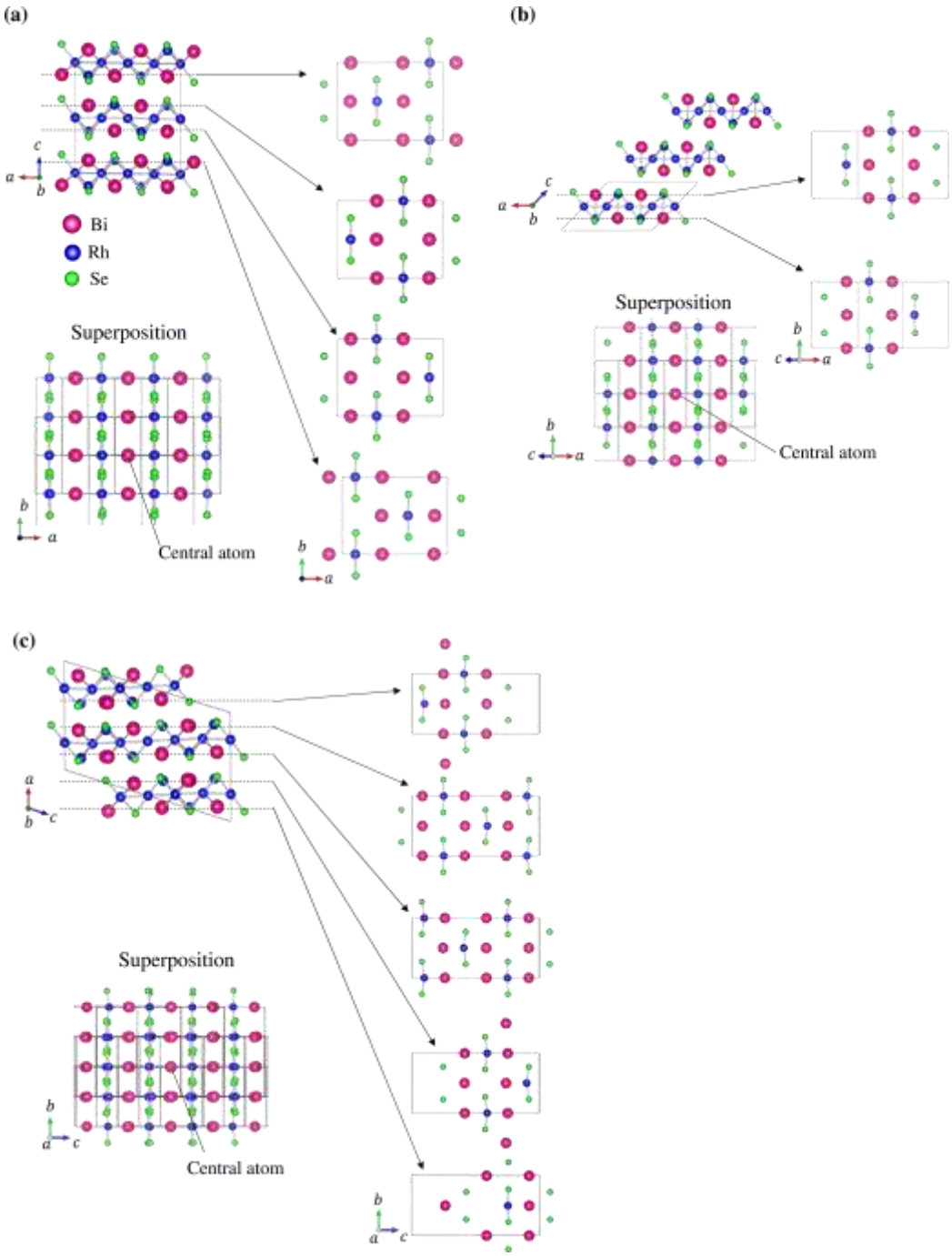

Figure S2. Schematic representations of (a) small β-cell, (b) large β-cell and (c) supercell structures. The used atomic coordinates and lattice constants are listed in Tables S1–S3 of Supporting Information. The reconstructed atomic image at z = 0 corresponds to the superposition of local atomic arrangements around Bi atoms in each model structure shown in (a) – (c); the local atomic arrangements are dawn within z ± 0.6 Å.

Table S1. Atomic coordinates used for preparation of small β-cell structure, which are taken from ref. 19. The lattice constants and space group (*C*2/*m* (No. 12)) taken from ref. 19 are a = 11.4316(7) Å, b = 8.3872(4) Å, c = 12.0157(3) Å, and β = 89.225(4)°.

atom	site	*x*	*y*	*z*
Bi(1)	4*i*	0.127(5)	0	0.384(2)
Bi(2)	4*i*	0.379(5)	0	0.119(2)
Bi(3)	4*i*	0.625(4)	0	0.390(2)
Bi(4)	4*i*	0.873(4)	0	0.112(2)
Rh(1)	4*e*	0.25	-0.25	0
Rh(2)	4*f*	0.25	0.25	0.5
Rh(3)	4*h*	0.5	-0.262(9)	0.5
Rh(4)	4*g*	1	-0.263(9)	0
Rh(5)	4*i*	0.372(2)	0	0.379(4)
Rh(6)	4*i*	0.124(2)	0	0.118(4)
Se(1)	8*j*	0.372(6)	-0.276(6)	0.332(2)
Se(2)	8*j*	0.129(6)	-0.278(5)	0.165(2)

Table S2. Atomic coordinates used for preparation of large β-cell structure, which are taken from the atomic coordinates at 293 K listed in Table II of ref. 23. The lattice constants of $Bi_2Rh_3Se_2$ (large β-cell structure) shown in ref. 18 are *a* = 11.413(1) Å, *b* = 8.368(2) Å, *c* = 8.336(1) Å and β = 134.05(4)°. The space group is assumed as *C*2/*m* (No. 12). Here, the S atom in the atomic coordinates listed in ref. 23 is replaced by Se.

atom	site	*x*	*y*	*z*
Bi(1)	4*i*	0.0002(1)	0	0.2518(2)
Bi(2)	4*i*	0.5086(1)	0	0.2596(2)
Rh(1)	4*f*	0.25	0.25	0.5
Rh(2)	4i	0.2472(1)	0	0.2472(2)
Rh(3)	4h	0	0.2411(2)	0.5
Se(2)	8j	0.2235(6)	0.2704(5)	0.187(1)

Table S3. Atomic coordinates used for preparation of supercell structure, which are taken from the atomic coordinates of $Bi_2Rh_3S_2$ listed in Table II of ref. 23. The lattice constants are converted to $Bi_2Rh_3Se_2$ from the lattice constants of $Bi_2Rh_3S_2$ (supercell structure) at 120 K listed in Table I of ref. 23; a = 11.6667 Å, b = 8.331 Å, c = 18.6495 Å and β = 107.614°. The space group is assumed as $C2/m$ (No. 12). Here, the S atom in the atomic coordinates listed in ref. 23 is replaced by Se.

atom	site	x	y	z
Bi(1)	4*i*	0.0709(1)	0	0.4167(1)
Bi(2)	4*i*	0.2432(1)	0	0.2599(1)
Bi(3)	4*i*	0.4026(1)	0	0.0830(1)
Bi(4)	4*i*	0.5778(1)	0	0.4148(1)
Bi(5)	4*i*	0.7383(1)	0	0.2464(1)
Bi(6)	4*i*	0.9041(1)	0	0.0831(1)
Rh(1)	8*j*	0.3196(2)	0.2470(3)	0.1674(1)
Rh(2)	8*j*	0.4092(2)	0.2517(3)	0.3347(1)
Rh(3)	4*i*	0.1550(3)	0	0.0983(1)
Rh(4)	4*i*	0.1802(3)	0	0.5923(2)
Rh(5)	4*i*	0.4860(3)	0	0.2499(2)
Rh(6)	4*h*	0	0.2670(5)	0.5
Rh(7)	4*e*	0.25	0.25	0
Se(1)	8*j*	0.0187(6)	0.2265(10)	0.2464(4)
Se(2)	8*j*	0.1262(6)	0.2706(10)	0.0806(4)
Se(3)	8*j*	0.3000(6)	0.2299(9)	0.4232(4)