Acta Crystallographica Section B

Volume 70 (2014)

Supporting information for article:

The quasiperiodic average structure of highly disordered decagonal Zn–Mg–Dy and its temperature dependence

Taylan Ors, Hiroyuki Takakura, Eiji Abe and Walter Steurer

Table S1 Table of refined parameters for the room-temperature dataset for the high-temperature experiments

Sub OD no.	Pre defined OD shape	x^i (perp. space component of the given vector)	u_1 (Å)	x^e_2 (par. space component of the given vector)	u_2 (Å)	x^e_3 (par. space component of the given vector)	u_3 (Å)	b_e (Å^2)	p	s_1	Element
OD1: x_0= 0. 0. 0. 0. 0.5 (in 5D basis setting)											
1	a	0. 0. 0. 0. 0. 0	0.26(3)	-	-	-	-	0.07(26)	0.50(-)	1.00(-)	Mg/Dy
2	b	0. 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.17(2)	-	-	0.07(26)	1.00(-)	1.00(-)	Mg/Dy
3	h	0. -0.618 0. 0.618 0. 0.	-	0. -1. 0. 1. 0. 0	0.01(31)	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
4	d	0. 0. 0. 0. -0.691 0.	-	0. 0. 0. 0. -1. 0.	0.01(31)	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
5	b	0. 0. 0. 0. -1. 0.	-	0. 0. 0. 0. -1. 0.	0.01(26)	-	-	0.67(22)	1.00(-)	0.23(18)	Zn/Mg
6	d	0. -0.809 0. 0.809 0. 0.	-	0. -1. 0. 1. 0. 0.	0.01(31)	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
7	e	0. -1. 0. 1. 0. 0.	-	0. -1. 0. 1. 0. 0.	-0.34(5)	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
8	b	0. 0. 0. 0. -1.236 0.	-	0. 0. 0. 0. -1. 0.	0.52(28)	-	-	0.71(37)	1.00(-)	1.00(2)	Zn/Mg
9	b	0. 0. 0. -0.236 -1.618 0	-	0. 0. 0. 0. -1. 0.	0.58(15)	0. -1. 1. 0. 0. 0.	-0.25(10)	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
10	b	0. -1. 0. 1. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.53(16)	0. -1. 1. 0. 0. 0.	0.08(6)	0.67(22)	1.00(-)	0.10(10)	Zn/Mg
11	j	0. 0. 0. 0. -1.618 0.	-	0. 0. 0. 0. -1. 0	0.52(79)	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg

12	i	0. 0. 0. 0. -1.764 0.	-	0. 0. 0. 0. -1. 0	0.57(66)	-	-	0.67(22)	1.00(-)	0.00(-)	Zn/Mg
13	b	0. -0.236 0. 0. -1.618 0.	-	0. 0. 0. 0. -1. 0.	0.56(33)	0. -1. 1. 0. 0. 0.	0.05(9)	0.67(22)	1.00(-)	0.00(-)	Zn/Mg
14	a	0. -1.618 0. 1.618 0. 0.	-	0. -1. 0. 1. 0. 0	-0.29(2)	-	-	0.67(22)	0.30(-)	0.00(-)	Zn/Mg
OD2: x_0 = 0.2 0.2 0.2 0.2 0.25 (in 5D basis setting)											
15	b	0. 0. 0. 0. 0. 0.	0.25(27)	-	-	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
16	f	0. 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.09(3)	-	-	0.57(32)	1.00(-)	0.00(-)	Zn/Mg
17	d	0.309 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-0.09(130)	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
18	b	0.618 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-0.20(7)	-	-	0.46(120)	1.00(-)	0.34(11)	Zn/Mg
19	b	0.382 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	-0.09(10)	0. -1. 1. 0. 0. 0.	0.00(3)	0.46(120)	1.00(-)	0.00(-)	Zn/Mg
21	a	1. 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-	-	-	3.24(121)	0.30(-)	0.00(-)	Zn/Mg
22	i	0. 0. 0. 0. -0.764 0.	-	0. 0. 0. 0. -1 0.	-0.07(27)	-	-	0.98(378)	1.00(-)	0.00(-)	Zn/Mg
OD4: x_0 = 0.4 0.4 0.4 0.4 0. (in 5D basis setting)											
24	c	0. 0. 0. 0. 0. 0.	-	-	-	-	-	0.33(36)	1.00(-)	0.00(-)	Zn/Mg
OD3: x_0 = 0.4 0.4 0.4 0.4 0.25 (in 5D basis setting)											
25	b	0.236 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	0.11(4)	-	-	0.25(36)	1.00(-)	0.00(-)	Zn/Mg
OD4: x_0 = 0.4 0.4 0.4 0.4 0. (in 5D basis setting)											
29	b	0. 0. 0. 0. -0.382 0.	-0.83(19)	0. 0. 0. 0. -1. 0.	0.09(34)	-	-	0.71(37)	0.50(-)	1.00(-)	Zn/Mg

30	a	0.618 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	0.29(4)	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
31	c	0. 0. 0. 0. -1. 0.	-	0. 0. 0. 0. -1. 0.	0.01(3)	-	-	0.33(36)	1.00(-)	0.00(-)	Zn/Mg
32	b	0. 0. 0. 0. -0.618 0.	-	0. 0. 0. 0. -1. 0.	0.15(4)	-	-	0.33(36)	1.00(-)	0.00(-)	Zn/Mg
33	b	0. 0. 0. -0.236 -1. 0.	-0.55(16)	0. 0. 0. 0. -1. 0.	-0.16(20)	0. -1. 1. 0. 0. 0.	-0.34(14)	0.71(37)	0.50(-)	1.00(-)	Zn/Mg
OD5: x_0 = 0. 0.5 0.5 0. 0. (in 5D basis setting)											
34	d	0. 0. 0. 0. 0. 0.	-	-	-		-	0.39(32)	1.00(-)	0.94(106)	Zn/Mg
35	e	0. -0.118 0.118 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	0.04(3)		-	0.39(32)	1.00(-)	0.00(-)	Zn/Mg
36	b	0. 0. 0. 0. -0.309 0.	-	0. 0. 0. 0. -1. 0.	-0.08(35)	-	-	0.71(37)	1.00(-)	1.00(-)	Zn/Mg
37	b	0. -0.118 0.118 0. -0.382 0.	-	0. -1. 1. 0. 0. 0.	0.12(6)	0. 0. 0. 0. -1. 0.	-0.01(6)	0.31(44)	1.00(-)	0.00(-)	Zn/Mg
38	b	0.382 -0.118 0.118 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	-0.11(4)	0. 0. 0. 0. -1. 0.	0.00(5)	0.31(44)	1.00(-)	0.00(-)	Zn/Mg
39	b	0. -0.309 0.309 0. -0.118 0.	-0.31(5)	0. -1. 1. 0. 0. 0.	0.03(5)	0. 0. 0. 0. -1. 0.	-0.11(7)	0.39(32)	0.50(-)	0.00(-)	Zn/Mg
40	b	0. -0.5 0.5 0.382 0. 0.	-	0. -1. 1. 0. 0. 0.	0.21(4)	0. 0. 0. 0. -1. 0.	0.16(5)	0.39(32)	0.50(-)	0.00(-)	Zn/Mg
41	a	0. -0.5 0.5 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	-0.14(9)	-	-	0.71(37)	0.30(-)	1.00(-)	Zn/Mg

Additional Parameters

Scale: 2.25994(3000) Extinction Parameter: -0.04654(3908) Mosaicity: 0.03000°(-) B_{Ph}=3.0566(2690) Å

Table S2 Table of refined parameters for the dataset measured at 325°C for the high-temperature experiments

Sub OD no.	Pre defined OD shape	x^i (perp. space component of the given vector)	u_1 (Å)	x^e_2 (par. space component of the given vector)	u_2 (Å)	x^e_3 (par. space component of the given vector)	u_3 (Å)	b_e (Å^2)	p	s_1	Element
OD1: x_0= 0. 0. 0. 0. 0.5 (in 5D basis setting)											
1	a	0. 0. 0. 0. 0. 0	0.31(3)	-	-	-	-	0.23(27)	0.50(-)	1.00(-)	Mg/Dy
2	b	0. 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.16(2)	-	-	0.23(27)	1.00(-)	1.00(-)	Mg/Dy
3	h	0. -0.618 0. 0.618 0. 0.	-	0. -1. 0. 1. 0. 0	0.12(10)	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
4	d	0. 0. 0. 0. -0.691 0.	-	0. 0. 0. 0. -1. 0.	0.12(10)	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
5	b	0. 0. 0. 0. -1. 0.	-	0. 0. 0. 0. -1. 0.	0.06(11)	-	-	1.59(26)	1.00(-)	0.16(29)	Zn/Mg
6	d	0. -0.809 0. 0.809 0. 0.	-	0. -1. 0. 1. 0. 0.	0.12(10)	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
7	e	0. -1. 0. 1. 0. 0.	-	0. -1. 0. 1. 0. 0.	-0.42(6)	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
8	b	0. 0. 0. 0. -1.236 0.	-	0. 0. 0. 0. -1. 0.	0.47(70)	-	-	1.82(46)	1.00(-)	0.97(29)	Zn/Mg
9	b	0. 0. 0. -0.236 -1.618 0	-	0. 0. 0. 0. -1. 0.	0.49(138)	0. -1. 1. 0. 0. 0.	-0.25(10)	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
10	b	0. -1. 0. 1. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.54(14)	0. -1. 1. 0. 0. 0.	0.08(6)	1.59(26)	1.00(-)	0.00(2)	Zn/Mg
11	j	0. 0. 0. 0. -1.618 0.	-	0. 0. 0. 0. -1. 0	0.52(312)	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
12	i	0. 0. 0. 0. -1.764 0.	-	0. 0. 0. 0. -1. 0	0.57(34)	-	-	1.59(26)	1.00(-)	0.00(-)	Zn/Mg

13	b	0. -0.236 0. 0. -1.618 0.	-	0. 0. 0. 0. -1. 0.	0.56(20)	0. -1. 1. 0. 0. 0.	0.05(9)	1.59(26)	1.00(-)	0.00(-)	Zn/Mg
14	a	0. -1.618 0. 1.618 0. 0.	-	0. -1. 0. 1. 0. 0	-0.28(3)	-	-	1.59(26)	0.30(-)	0.00(-)	Zn/Mg
OD2: x_0 = 0.2 0.2 0.2 0.2 0.25 (in 5D basis setting)											
15	b	0. 0. 0. 0. 0. 0.	0.36(30)	-	-	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
16	f	0. 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.13(1)	-	-	1.18(19)	1.00(-)	0.00(-)	Zn/Mg
17	d	0.309 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-0.01(389)	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
18	b	0.618 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-0.26(6)	-	-	1.31(96)	1.00(-)	0.39(13)	Zn/Mg
19	b	0.382 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	-0.09(30)	0. -1. 1. 0. 0. 0.	0.00(3)	1.31(96)	1.00(-)	0.00(-)	Zn/Mg
21	a	1. 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-	-	-	5.92(178)	0.30(-)	0.00(-)	Zn/Mg
22	i	0. 0. 0. 0. -0.764 0.	-	0. 0. 0. 0. -1 0.	-0.10(58)	-	-	1.11(227)	1.00(-)	0.00(-)	Zn/Mg
OD4: x_0 = 0.4 0.4 0.4 0.4 0. (in 5D basis setting)											
24	c	0. 0. 0. 0. 0. 0.	-	-	-	-	-	1.15(32)	1.00(-)	0.00(-)	Zn/Mg
OD3: x_0 = 0.4 0.4 0.4 0.4 0.25 (in 5D basis setting)											
25	b	0.236 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	0.11(5)	-	-	1.24(47)	1.00(-)	0.00(-)	Zn/Mg
OD4: x_0 = 0.4 0.4 0.4 0.4 0. (in 5D basis setting)											
29	b	0. 0. 0. 0. -0.382 0.	-0.89(25)	0. 0. 0. 0. -1. 0.	-0.17(35)	-	-	1.82(46)	0.50(-)	1.00(-)	Zn/Mg
30	a	0.618 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	0.33(5)	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg

31	c	0. 0. 0. 0. -1. 0.	-	0. 0. 0. 0. -1. 0.	0.12(4)	-	-	1.15(32)	1.00(-)	0.00(-)	Zn/Mg
32	b	0. 0. 0. 0. -0.618 0.	-	0. 0. 0. 0. -1. 0.	0.00(9)	-	-	1.15(32)	1.00(-)	0.00(-)	Zn/Mg
33	b	0. 0. 0. -0.236 -1. 0.	-0.62(21)	0. 0. 0. 0. -1. 0.	-0.17(27)	0. -1. 1. 0. 0. 0.	-0.34(14)	1.82(46)	0.50(-)	1.00(-)	Zn/Mg
OD5: x_0 = 0. 0.5 0.5 0. 0. (in 5D basis setting)											
34	d	0. 0. 0. 0. 0. 0.	-	-	-		-	0.98(28)	1.00(-)	1.00(2)	Zn/Mg
35	e	0. -0.118 0.118 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	0.02(2)		-	0.98(28)	1.00(-)	0.00(-)	Zn/Mg
36	b	0. 0. 0. 0. -0.309 0.	-	0. 0. 0. 0. -1. 0.	-0.07(37)	-	-	1.82(46)	1.00(-)	1.00(-)	Zn/Mg
37	b	0. -0.118 0.118 0. -0.382 0.	-	0. -1. 1. 0. 0. 0.	0.18(4)	0. 0. 0. 0. -1. 0.	-0.01(6)	0.80(41)	1.00(-)	0.00(-)	Zn/Mg
38	b	0.382 -0.118 0.118 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	-0.16(3)	0. 0. 0. 0. -1. 0.	0.00(5)	0.80(41)	1.00(-)	0.00(-)	Zn/Mg
39	b	0. -0.309 0.309 0. -0.118 0.	-0.48(6)	0. -1. 1. 0. 0. 0.	-0.01(5)	0. 0. 0. 0. -1. 0.	-0.11(7)	0.98(28)	0.50(-)	0.00(-)	Zn/Mg
40	b	0. -0.5 0.5 0.382 0. 0.	-	0. -1. 1. 0. 0. 0.	0.21(4)	0. 0. 0. 0. -1. 0.	0.16(5)	0.98(28)	0.50(-)	0.00(-)	Zn/Mg
41	a	0. -0.5 0.5 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	-0.07(11)	-	-	1.82(46)	0.30(-)	1.00(-)	Zn/Mg

Additional Parameters

Scale: 2.23407(3272) Extinction Parameter: 0.01357(5959) Mosaicity: 0.03000°(-) B_{Ph}=2.5891(2596) Å

Table S3 Table of refined parameters for the dataset measured at 375°C for the high-temperature experiments

Sub OD no.	Pre defined OD shape	x^i (perp. space component of the given vector)	u_1 (Å)	x^e_2 (par. space component of the given vector)	u_2 (Å)	x^e_3 (par. space component of the given vector)	u_3 (Å)	b_e (Å^2)	p	s_1	Element
OD1: x_0= 0. 0. 0. 0. 0.5 (in 5D basis setting)											
1	a	0. 0. 0. 0. 0. 0	0.31(3)	-	-	-	-	0.65(30)	0.50(-)	1.00(-)	Mg/Dy
2	b	0. 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.14(3)	-	-	0.65(30)	1.00(-)	1.00(-)	Mg/Dy
3	h	0. -0.618 0. 0.618 0. 0.	-	0. -1. 0. 1. 0. 0	0.16(5)	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
4	d	0. 0. 0. 0. -0.691 0.	-	0. 0. 0. 0. -1. 0.	0.16(5)	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
5	b	0. 0. 0. 0. -1. 0.	-	0. 0. 0. 0. -1. 0.	0.08(5)	-	-	1.80(24)	1.00(-)	0.00(2)	Zn/Mg
6	d	0. -0.809 0. 0.809 0. 0.	-	0. -1. 0. 1. 0. 0.	0.16(5)	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
7	e	0. -1. 0. 1. 0. 0.	-	0. -1. 0. 1. 0. 0.	-0.39(7)	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
8	b	0. 0. 0. 0. -1.236 0.	-	0. 0. 0. 0. -1. 0.	0.48(53)	-	-	2.54(48)	1.00(-)	0.82(20)	Zn/Mg
9	b	0. 0. 0. -0.236 -1.618 0	-	0. 0. 0. 0. -1. 0.	0.49(122)	0. -1. 1. 0. 0. 0.	-0.25(10)	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
10	b	0. -1. 0. 1. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.55(10)	0. -1. 1. 0. 0. 0.	0.08(6)	1.80(24)	1.00(-)	0.00(2)	Zn/Mg
11	j	0. 0. 0. 0. -1.618 0.	-	0. 0. 0. 0. -1. 0	0.51(260)	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg

12	i	0. 0. 0. 0. -1.764 0.	-	0. 0. 0. 0. -1. 0	0.59(22)	-	-	1.80(24)	1.00(-)	0.00(-)	Zn/Mg
13	b	0. -0.236 0. 0. -1.618 0.	-	0. 0. 0. 0. -1. 0.	0.56(13)	0. -1. 1. 0. 0. 0.	0.05(9)	1.80(24)	1.00(-)	0.00(-)	Zn/Mg
14	a	0. -1.618 0. 1.618 0. 0.	-	0. -1. 0. 1. 0. 0	-0.29(2)	-	-	1.80(24)	0.30(-)	0.00(-)	Zn/Mg
OD2: x_0 = 0.2 0.2 0.2 0.2 0.25 (in 5D basis setting)											
15	b	0. 0. 0. 0. 0. 0.	0.35(31)	-	-	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
16	f	0. 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	0.14(2)	-	-	1.52(22)	1.00(-)	0.00(-)	Zn/Mg
17	d	0.309 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-0.02(357)	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
18	b	0.618 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-0.27(7)	-	-	1.48(107)	1.00(-)	0.50(11)	Zn/Mg
19	b	0.382 0. 0. 0. -0.382 0.	-	0. 0. 0. 0. -1. 0.	-0.10(16)	0. -1. 1. 0. 0. 0.	0.00(3)	1.48(107)	1.00(-)	0.00(-)	Zn/Mg
21	a	1. 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	-	-	-	6.42(157)	0.30(-)	0.00(-)	Zn/Mg
22	i	0. 0. 0. 0. -0.764 0.	-	0. 0. 0. 0. -1 0.	-0.09(35)	-	-	1.70(301)	1.00(-)	0.00(-)	Zn/Mg
OD4: x_0 = 0.4 0.4 0.4 0.4 0. (in 5D basis setting)											
24	c	0. 0. 0. 0. 0. 0.	-	-	-	-	-	1.48(37)	1.00(-)	0.00(-)	Zn/Mg
OD3: x_0 = 0.4 0.4 0.4 0.4 0.25 (in 5D basis setting)											
25	b	0.236 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	0.13(4)	-	-	1.50(45)	1.00(-)	0.00(-)	Zn/Mg
OD4: x_0 = 0.4 0.4 0.4 0.4 0. (in 5D basis setting)											
29	b	0. 0. 0. 0. -0.382 0.	-0.93(24)	0. 0. 0. 0. -1. 0.	-0.02(118)	-	-	2.54(48)	0.50(-)	1.00(-)	Zn/Mg

30	a	0.618 0. 0. 0. 0. 0.	-	1. 0. 0. 0. 0. 0.	0.31(4)	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
31	c	0. 0. 0. 0. -1. 0.	-	0. 0. 0. 0. -1. 0.	0.12(3)	-	-	1.48(37)	1.00(-)	0.00(-)	Zn/Mg
32	b	0. 0. 0. 0. -0.618 0.	-	0. 0. 0. 0. -1. 0.	-0.05(8)	-	-	1.48(37)	1.00(-)	0.00(-)	Zn/Mg
33	b	0. 0. 0. -0.236 -1. 0.	-0.72(17)	0. 0. 0. 0. -1. 0.	-0.04(32)	0. -1. 1. 0. 0. 0.	-0.34(14)	2.54(48)	0.50(-)	1.00(-)	Zn/Mg
OD5: x_0 = 0. 0.5 0.5 0. 0. (in 5D basis setting)											
34	d	0. 0. 0. 0. 0. 0.	-	-	-		-	1.44(22)	1.00(-)	1.00(2)	Zn/Mg
35	e	0. -0.118 0.118 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	0.06(4)		-	1.44(22)	1.00(-)	0.00(-)	Zn/Mg
36	b	0. 0. 0. 0. -0.309 0.	-	0. 0. 0. 0. -1. 0.	0.00(67)	-	-	2.54(48)	1.00(-)	1.00(-)	Zn/Mg
37	b	0. -0.118 0.118 0. -0.382 0.	-	0. -1. 1. 0. 0. 0.	0.10(8)	0. 0. 0. 0. -1. 0.	-0.01(6)	1.26(34)	1.00(-)	0.00(-)	Zn/Mg
38	b	0.382 -0.118 0.118 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	-0.19(2)	0. 0. 0. 0. -1. 0.	0.00(5)	1.26(34)	1.00(-)	0.00(-)	Zn/Mg
39	b	0. -0.309 0.309 0. -0.118 0.	-0.45(5)	0. -1. 1. 0. 0. 0.	0.01(5)	0. 0. 0. 0. -1. 0.	-0.11(7)	1.44(22)	0.50(-)	0.00(-)	Zn/Mg
40	b	0. -0.5 0.5 0.382 0. 0.	-	0. -1. 1. 0. 0. 0.	0.17(5)	0. 0. 0. 0. -1. 0.	0.16(5)	1.44(22)	0.50(-)	0.00(-)	Zn/Mg
41	a	0. -0.5 0.5 0. 0. 0.	-	0. -1. 1. 0. 0. 0.	-0.14(11)	-	-	2.54(48)	0.30(-)	1.00(-)	Zn/Mg

Additional Parameters

Scale: 2.05022(2659) Extinction Parameter: 0.06080(5998) Mosaicity: 0.03000°(-) B_{Ph}=3.30062(2322) Å

Approximation to the trend line slopes observed in log(*I*/*I*) vs. H_{perp}^2 graphs

The ratios of the observed intensities can be approximated by:

$$\frac{I_{\mathrm{T1}}}{I_{\mathrm{T2}}} = \frac{|F_{\mathrm{T1}}|^2}{|F_{\mathrm{T2}}|^2} \cong \frac{[e^{-\frac{B_{\mathrm{ph}}^{\mathrm{T1}}}{4}\times H_{\mathrm{perp}}^2} \times e^{-\frac{B_{\mathrm{par}}^{\mathrm{T1}}}{4}\times H_{\mathrm{par}}^2}]^2}{[e^{-\frac{B_{\mathrm{ph}}^{\mathrm{T2}}}{4}\times H_{\mathrm{perp}}^2} \times e^{-\frac{B_{\mathrm{par}}^{\mathrm{T2}}}{4}\times H_{\mathrm{par}}^2}]^2}$$

Where B_{par}^{T1} and B_{par}^{T2} represent an overall parallel space ADP factor at two given temperatures represented by *T1* and *T2*. Taking natural logarithm of both sides:

$$\ln\frac{I_{\mathrm{T1}}}{I_{\mathrm{T2}}} = -\frac{1}{2}\left(B_{\mathrm{ph}}^{\mathrm{T1}} - B_{\mathrm{ph}}^{\mathrm{T2}}\right) \times H_{\mathrm{perp}}^2 - \frac{1}{2}\left(B_{\mathrm{par}}^{\mathrm{T1}} - B_{\mathrm{par}}^{\mathrm{T2}}\right) \times H_{\mathrm{par}}^2$$

For a good comparison one can choose the temperatures closest to one another (T1=325°C and T2=375°C). Then for a first approximation, the two high temperature parallel space thermal motion terms, namely B_{par}^{325} and B_{par}^{375}, can be assumed to stay the same. This simplifies the equation to:

$$\ln\frac{I_{325}}{I_{375}} = -\frac{1}{2}\left(B_{\mathrm{ph}}^{325} - B_{\mathrm{ph}}^{375}\right) \times H_{\mathrm{perp}}^2$$

Which indicates a linear relationship between ln(*I*/*I*) and. H_{perp}^2 terms. Putting the refined values B_{par}^{325}=2.59 Å and B_{par}^{375}=3.30 Å, we obtain the value 0.36 Å for the slope. Converting the value obtained for the trend line in Fig.9i from log to ln basis we obtain a slope of 0.81 Å. These two values are significantly different due to approximations based on the average B_{par} value and that it stays constant between to different temperatures. However they point to a same trend in the graph and the fact that they are on the same order of magnitude might indicate that the main cause of change in the observed intensities is the change in B_{ph} values.

Figure S1 $\ln(I_{obs}/I_{calc})$ *versus* H_{perp}^2 plot (PILATUS data).

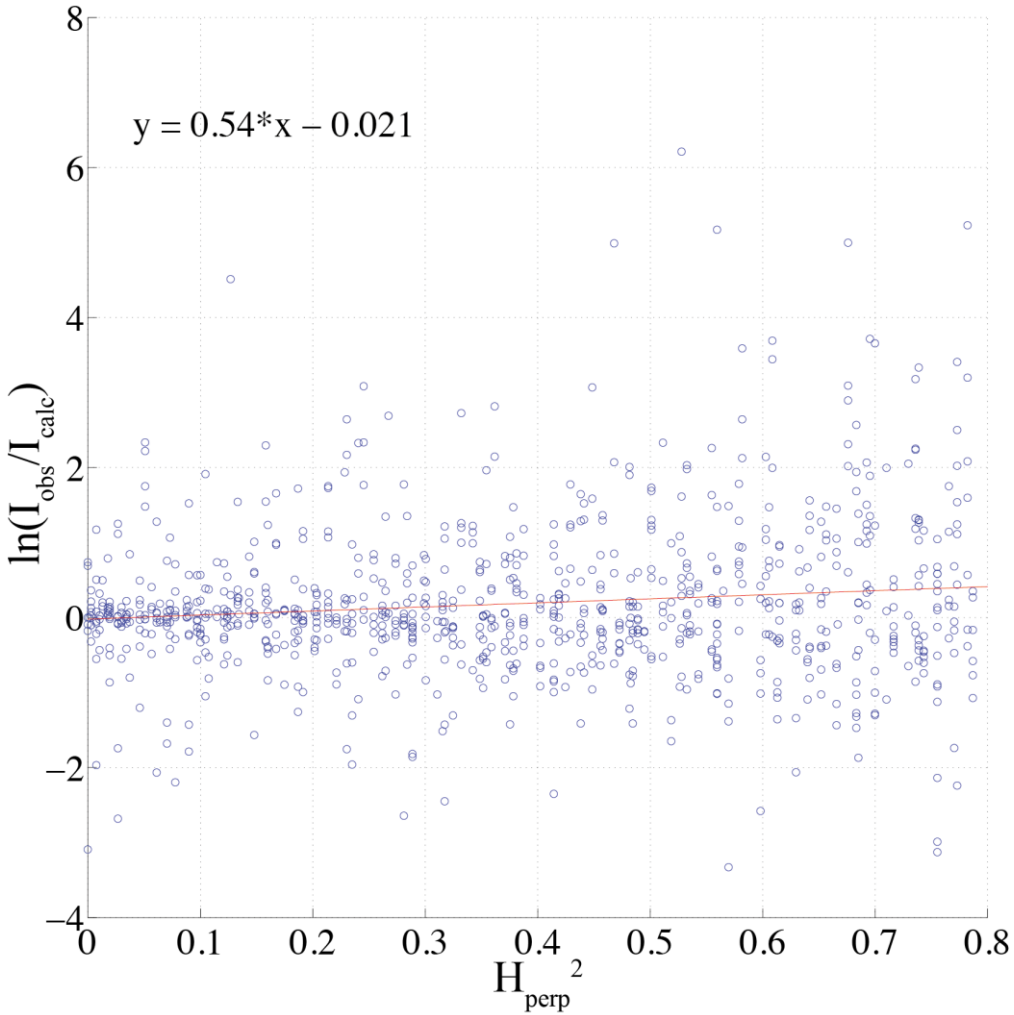


Figure S2 $\ln(I_{obs}/I_{calc})$ *versus* H_{par}^2 plot (PILATUS data).

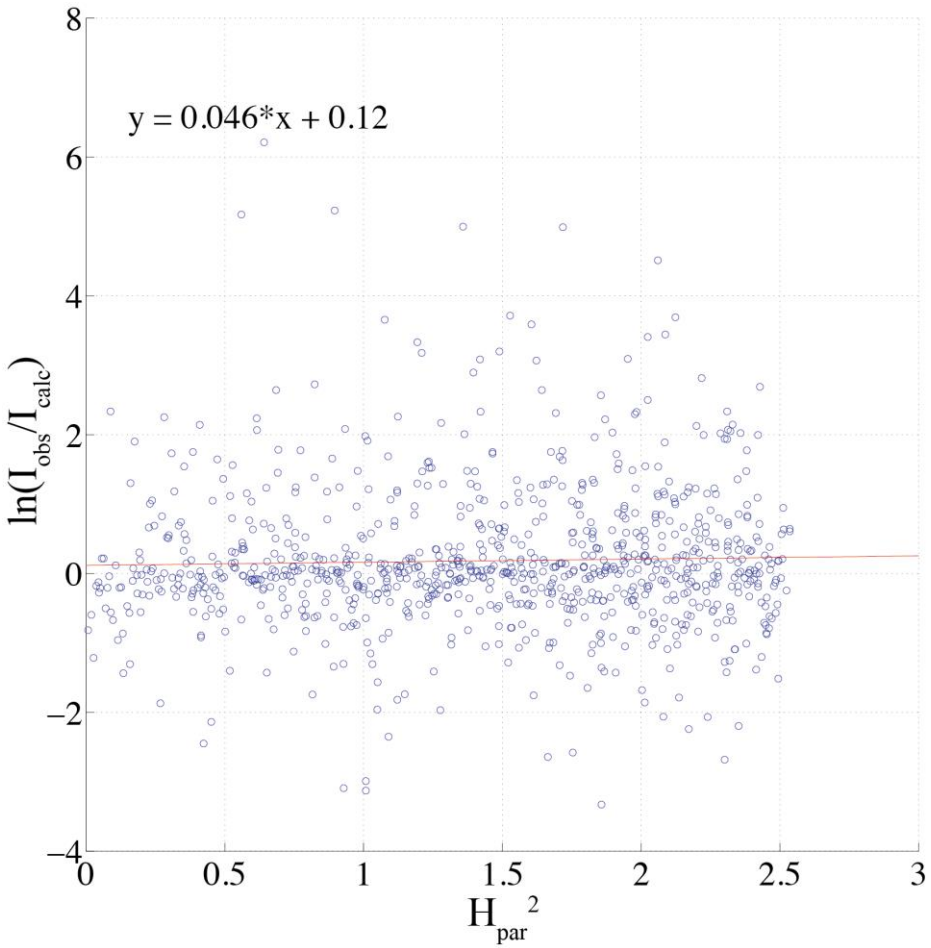
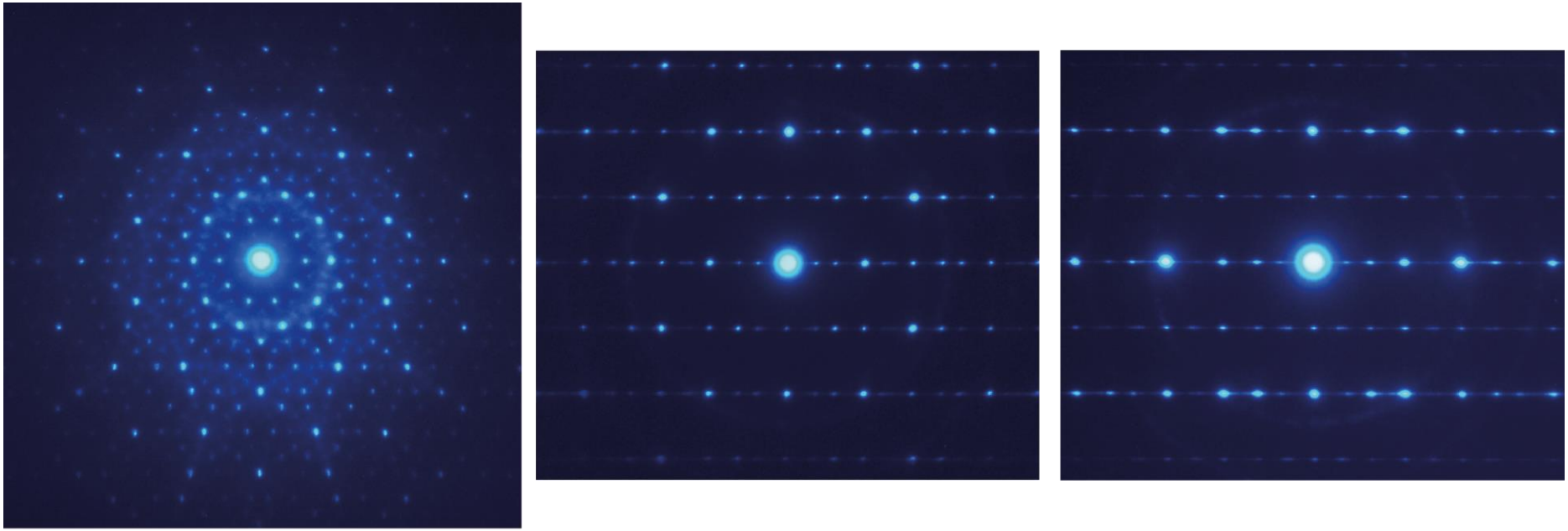


Figure S3 Electron diffraction image of the part of the d-ZnMgDy sample shown in the Z-contrast STEM image (Fig. 5).



(a) (b) (c)

Figure S4 Section of the five-dimensional unit cell that exhibits the edge center positions in the ideal penrose tiling. Red ODs are ideal PT and blue ODs generate all the possible tile edge center positions. The twofold shapes of the blue ODs (rhombs) are a consequence of the closeness condition.

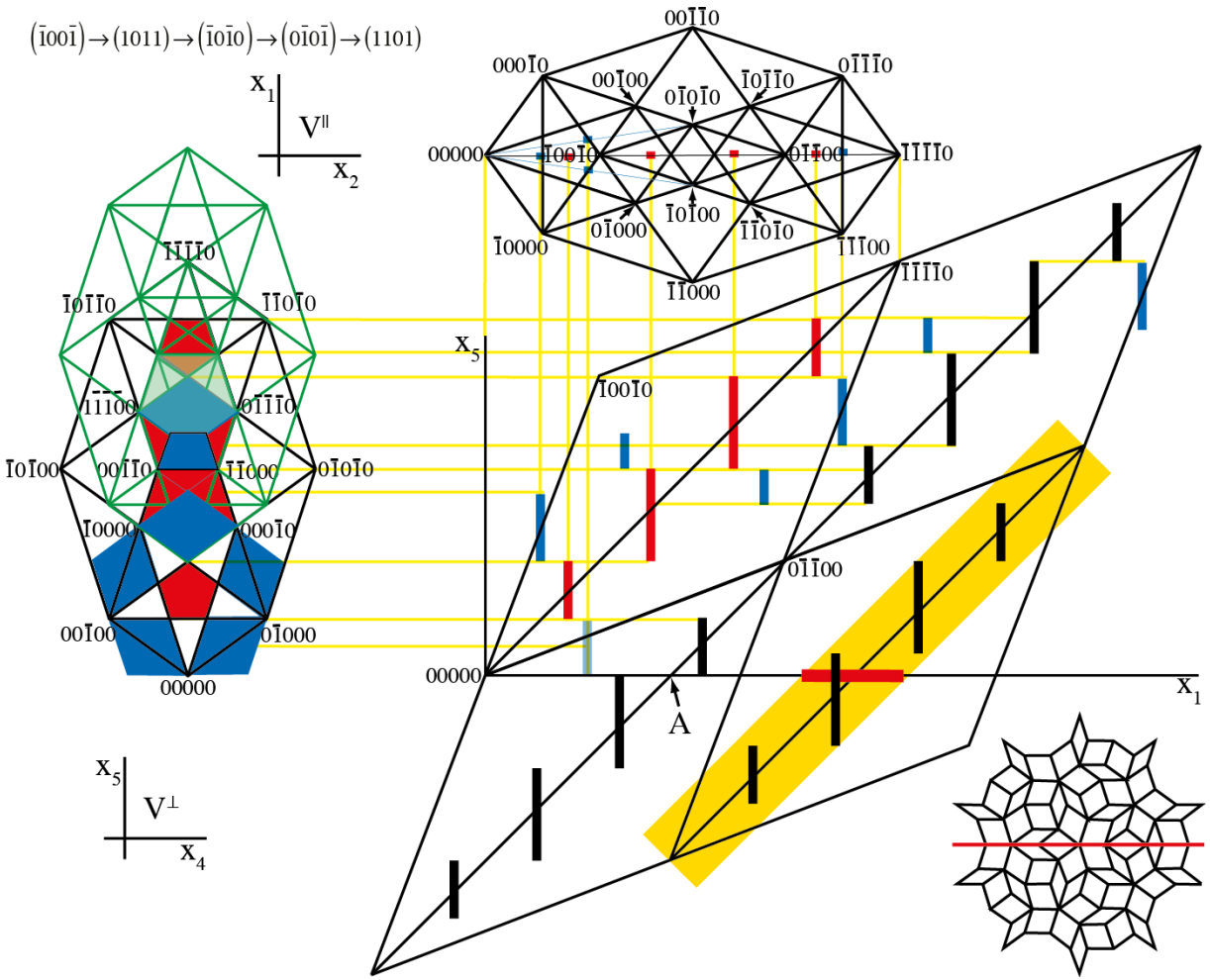


Figure S5 F_{obs} *versus* F_{calc} plot (CCD data)