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Supporting information for article:

Sphere packings as a tool for the description of martensitic phase transformations

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Supporting information

Group-subgroup relations are useful tools to describe relationships between structures if the space group of one compound is a subgroup of the space group of the other compound. If the space group under consideration is a general subgroup of a space group with higher symmetry, a series of maximal space groups have to be given in order to show the symmetry relations (*c.f. e.g.* International Tables vol. A1). In the case of martensitic phase transformations the specification of a chain of maximal subgroups does not imply that there are intermediate phases. Only the common subgroup allows deforming the structures into each other according to the pathway under consideration. The orientation relations between the unit cells of both structures may be obtained from the lattice vectors while from the indices of translationengleiche subgroups the number of twins (variants) can be deduced. Klassengleiche subgroups may lead to antiphase domains. Figures S1 to S5 show the symmetry relations between the phases as mentioned in the paper.

Since the true pathways describing the Nishiyama-Wassermann mechanism within the two-dimensional parameter region of sphere-packing type 8/4/*c*1 in *C*2/*m* 2*a* 0, 0, 0 can not be determined geometrically, the calculations were done keeping the four next nearest neighbours of each atom equidistant during the transformation. Table S1 gives parameter values for the NW1 and NW2 pathways in Fig. 4. The distance d_{cpp} between closest packed planes may by computed by d_{cpp} = $c_m\cos(\beta\text{-}90)$. Table S2 shows those for the Bain path. In this case the monoclinic angle is always β=135°. Table S3 shows structural parameters during the transformation according to the Kurdjumow-Sachs mechanism. The path through the two-dimensional parameter region of sphere-packing type 8/4/*c*1 was also calculated with four equidistant next nearest neighbours. The distance d_{cpp} between closest packed planes corresponds to $d_{(010)}$ of the triclinic unit cell. Structural parameters along the one-dimensional parameter region of sphere-packing type 8/4/*c*1 in *C*2/*m* 2*a* 0, 0 ,0 according to the Pitsch path are given in Table S4.

Tables S5 und S6 display the variations along the one-dimensional parameter regions of sphere packing types 11/3/*m*1 in *C*2/*m* 4*i x*, 0, *z* and 11/3/*h*2 in $P3_221$ 6*c x*, *y*, *z*, respectively. The distance between closest packed planes is defined by d_{cpp} = $\Delta zc\cos(90\text{-}\beta)$ in *C*2/*m* 4*i* and by d_{cpp} = Δzc in $P3_221$ 6*c*, where Δz is the difference between the *z* parameters of the atoms in adjacent planes. Details for the structural parameters during the transformation along the Pitsch-Schrader path between the *bcc* and *hcp* types are given by Sowa (2000*a*). Table S7 shows the corresponding parameter variations. Those according to the Burgers path are given in Table S8. Again the pathway is calculated under the condition that the four next nearest neighbours remain equidistant during the transformation. The distances between closest packed planes are d_{cpp} = $c_o/2$ in *Cmcm* 4*c* 0, *y*, 1/4 (Pitsch-Schrader path) and d_{cpp} = $b_m/2$ in $P2_1/m$ 2*e x*, 1/4, *z* (Burgers path).

Table S1 Variations of the structural parameters during the transformation between *bcc* and *fcc* types according to the Nishiyama-Wassermann path.

a_m	b_m	c_m (NW1)	c_m (NW2)	β (°) (NW1)	β (°) (NW2)	
1.63299	1.1547	1.1547	1.1547	135	135	*bcc*
1.64258	1.14103	1.14103	1.18157	134	136	
1.65232	1.12688	1.12688	1.20843	133	137	
1.66221	1.11223	1.11223	1.23526	132	138	
1.67224	1.09709	1.09709	1.26206	131	139	
1.68241	1.08143	1.08143	1.28880	130	140	
1.69270	1.06525	1.06525	1.31548	129	141	
1.70311	1.04854	1.04854	1.34207	128	142	
1.71361	1.03128	1.03128	1.36855	127	143	
1.72421	1.01346	1.01346	1.39491	126	144	
1.73205	1	1	1.41421	125.264	144.735	*fcc*

Table S2 Variations of the structural parameters during the transformation between *bcc* and *fcc* types according to the Bain path.

a_m	b_m	c_m	c/b	
1.63299	1.1547	1.1547	1	*bcc*
1.57267	1.23560	1.11204	0.9	
1.49854	1.32453	1.05963	0.8	
1.41421	1.41421	1	0.7071	*fcc*

Table S3 Variations of the structural parameters during the transformation between *bcc* and *fcc* types according to the Kurdjumow-Sachs path.

a_a	b_a	c_a	$\alpha = \beta$ (°)	γ (°)	
1	1	1.15470	125.264	70.529	*bcc*
1	1	1.11839	124	68	
1	1	1.08927	123	66	
1	1	1.05984	122	64	
1	1	1.03008	121	62	
1	1	1	120	60	*fcc*

Table S4 Variations of the structural parameters during the transformation between *bcc* and *fcc* types according to the Pitsch path.

a_m	b_m	c_m	β (°)	
1.15470	1.63299	1	125.264	*bcc*
1.17557	1.61803	1	126	
1.20363	1.59727	1	127	
1.23132	1.57602	1	128	
1.25864	1.55429	1	129	
1.28558	1.53209	1	130	
1.31212	1.50942	1	131	
1.33826	1.48629	1	132	
1.36400	1.46201	1	133	
1.38937	1.43868	1	134	
1.41421	1.41421	1	135	*fcc*

Table S5 Variations of the structural parameters during the transformation between *hcp* and *fcc* types according to the monoclinic path.

x	z	a_m	b_m	c_m	β (°)	
0.166667	0.25	1.73205	1	1.63299	90	*hcp*
0.17490	0.24725	1.73205	1	1.65215	92	
0.18315	0.24516	1.73205	1	1.66929	94	
0.19144	0.24371	1.73205	1	1.68440	96	
0.19979	0.24287	1.73205	1	1.69745	98	
0.20823	0.24265	1.73205	1	1.70844	100	
0.21677	0.24303	1.73205	1	1.71735	102	
0.22543	0.24403	1.73205	1	1.72416	104	
0.23425	0.24565	1.73205	1	1.72887	106	
0.24325	0.24791	1.73205	1	1.73148	108	
0.25	0.25	1.73205	1	1.73205	109.471	*fcc*

Table S6 Variations of the structural parameters during the transformation between *hcp* and *fcc* types according to the hexagonal path.

x	y	z	a_h	c_h	
0.33333	0.66667	.25	1	4.89898	*hcp*
0.35	0.66667	0.24951	1	4.92790	
0.4	0.66667	0.24840	1	4.99507	
0.45	0.66667	0.24776	1	5.03454	
0.5	0.66667	0.24755	1	5.04757	
0.55	0.66667	0.24776	1	5.03454	
0.6	0.66667	0.24840	1	4.99507	
0.65	0.66667	0.24951	1	4.92790	
0.66667	0.66667	0.25	1	4.89898	*fcc*

Table S7 Variations of the structural parameters during the transformation between *bcc* and *hcp* types according to the Pitsch-Schrader path.

y	a_o	b_o	c_o	
0.25	1.15470	1.63299	1.63299	*bcc*
0.24	1.13899	1.64399	1.64267	
0.23	1.12262	1.65521	1.64991	
0.22	1.10554	1.66667	1.65462	
0.21	1.08770	1.67836	1.65674	
0.20	1.06904	1.69031	1.65616	
0.19	1.04950	1.70251	1.65275	
0.18	1.02899	1.71499	1.64639	
0.17	1.00744	1.72774	1.63689	
0.166666	1	1.73205	1.63299	*hcp*

Table S8 Variations of the structural parameters during the transformation between *bcc* and *hcp* types according to the Burgers path.

x	z	a_m	b_m	c_m	β(°)	
0.75	0.5	1.154701	1.63299	1	125.264	*bcc*
0.72748	0.45496	1.11839	1.65133	1	124	
0.71087	0.42173	1.08928	1.65666	1	123	
0.69523	0.39046	1.05984	1.65489	1	122	
0.68051	0.36103	1.0301	1.64679	1	121	
0.66667	0.33333	1	1.63299	1	120	*hcp*

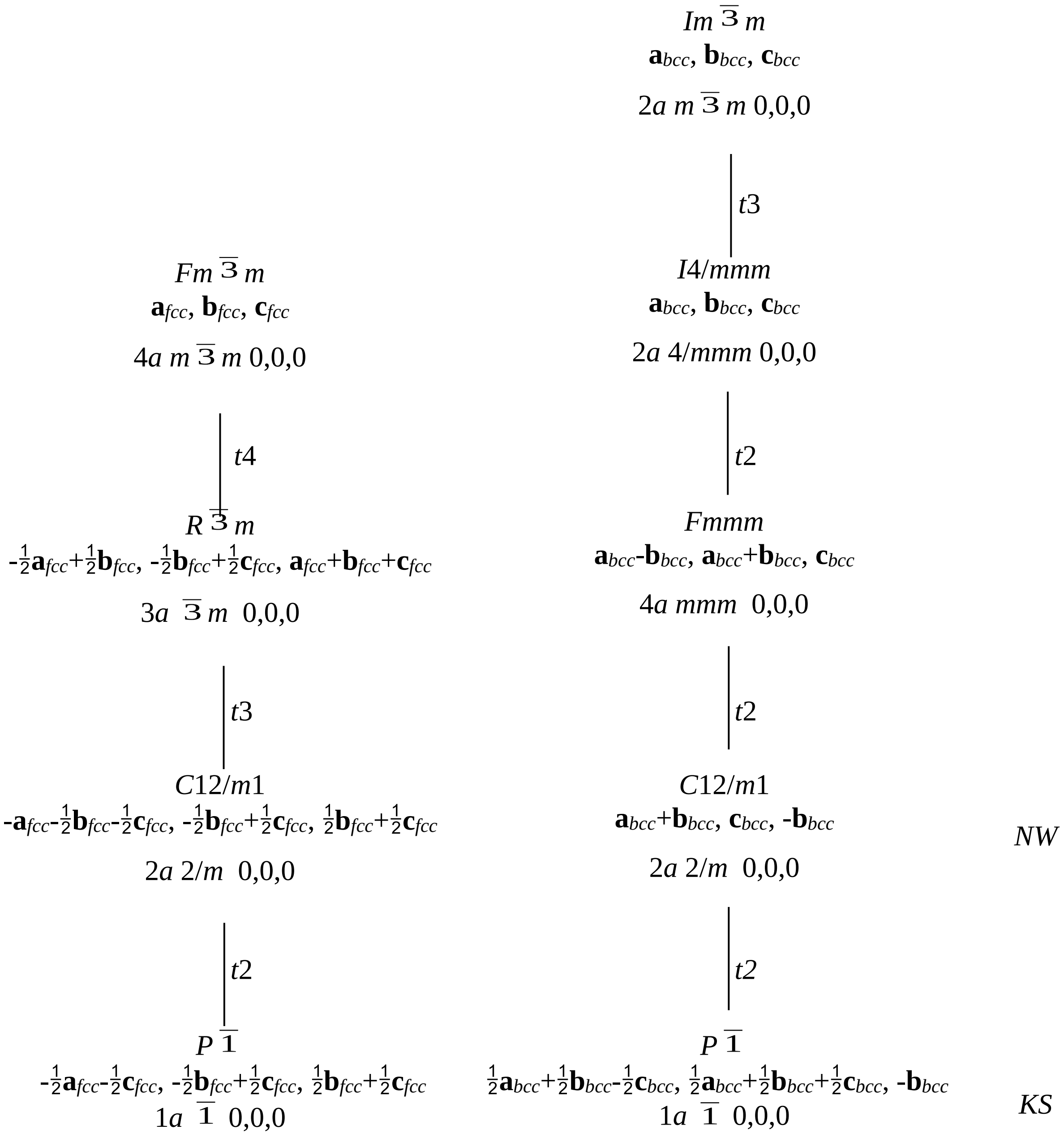

Figure S1 Symmetry relations between *fcc* and *bcc* type structures according to the Nishiyama-Wassermann (NW) and the Kurdjumow-Sachs (KS) path. The symbols *ti* indicate translationengleiche subgroups where *i* is the index of the subgroup.

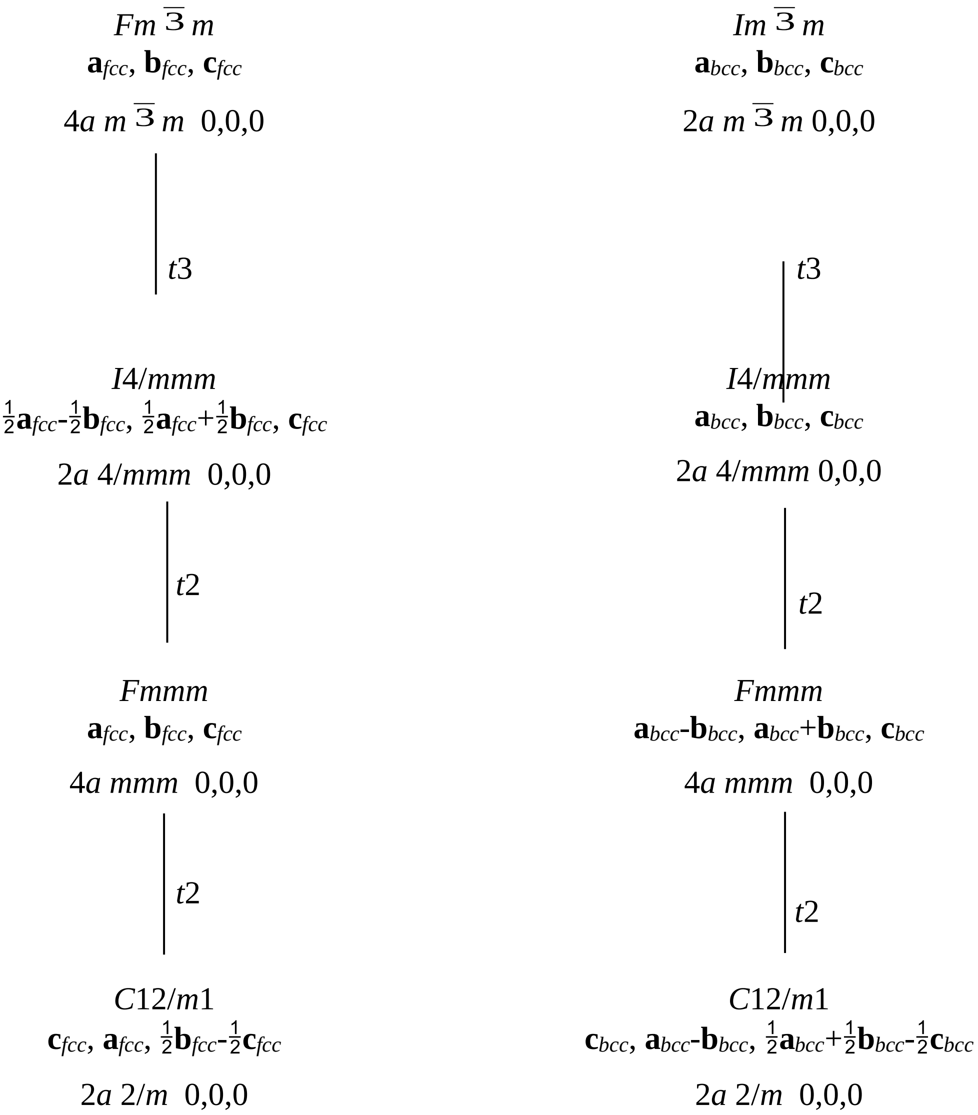

Fig. S2 Symmetry relations between *fcc* and *bcc* type structures according to the Pitsch mechanism. The symbols *ti* indicate translationengleiche subgroups where *i* is the index of the subgroup.

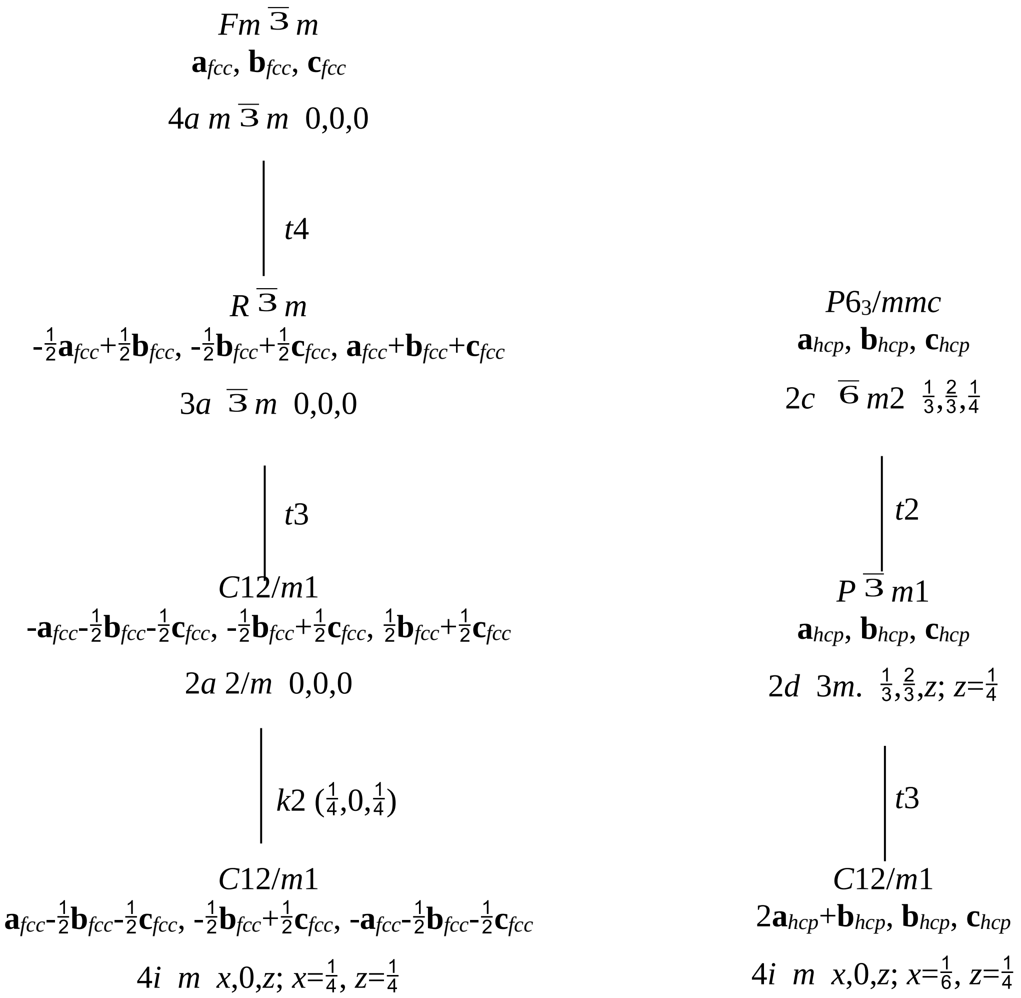

Figure S3 Symmetry relations between *fcc* and *hcp* type structures according to a monoclinic path. The symbols ti or ki indicate translationengleiche or klassengleiche subgroups, respectively. *i* is the index of the subgroup. The vector (1/4 0 1/4) specifies the shift of the origin that is necessary to obtain the standard description of the space group.

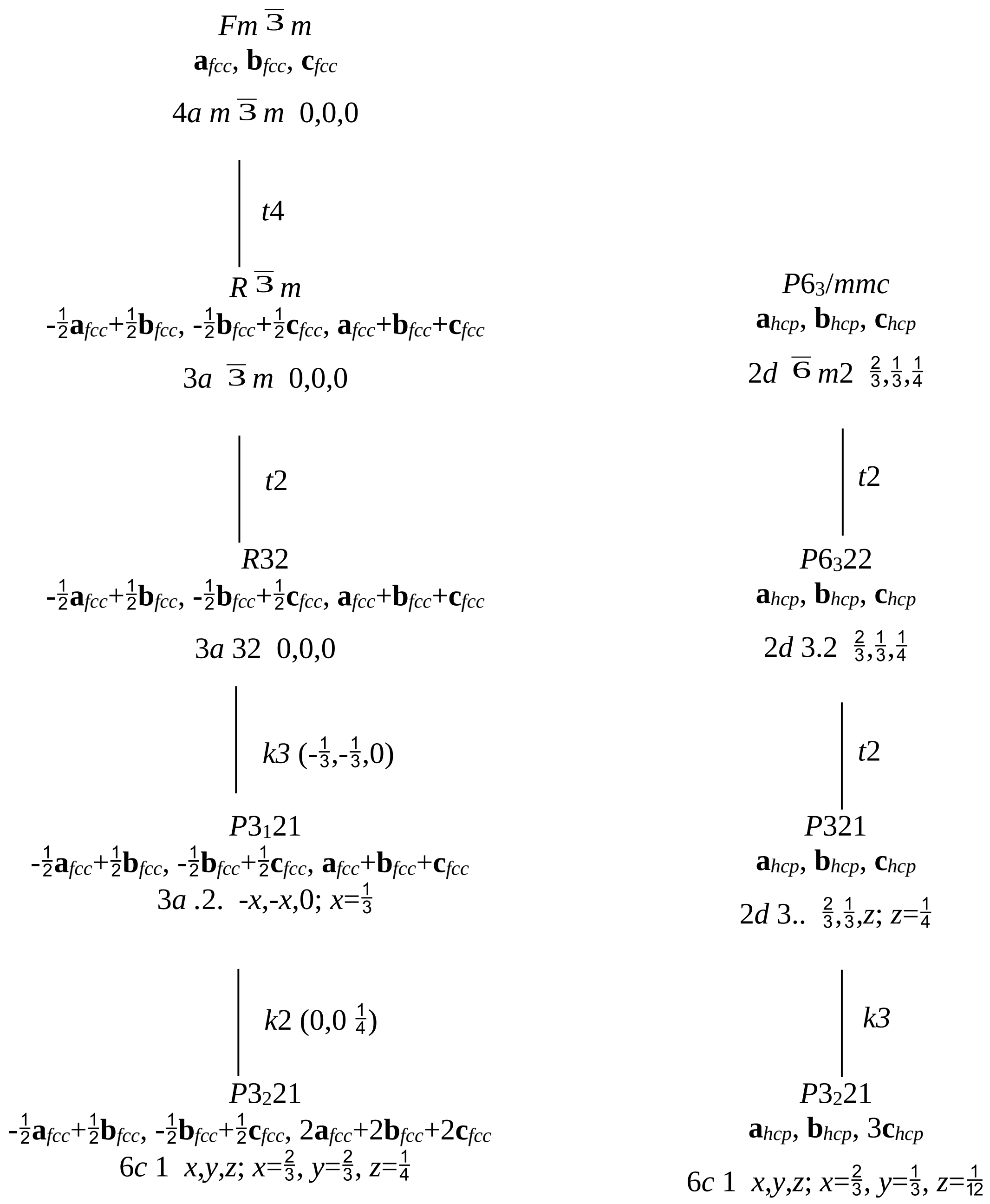

Figure S4 Symmetry relations between *fcc* and *hcp* type structures according to a trigonal path. The symbols ti or ki indicate translationengleiche or klassengleiche subgroups, respectively. *i* is the index of the subgroup. The vectors specify the shift of the origin that is necessary to obtain the standard description of the space group.

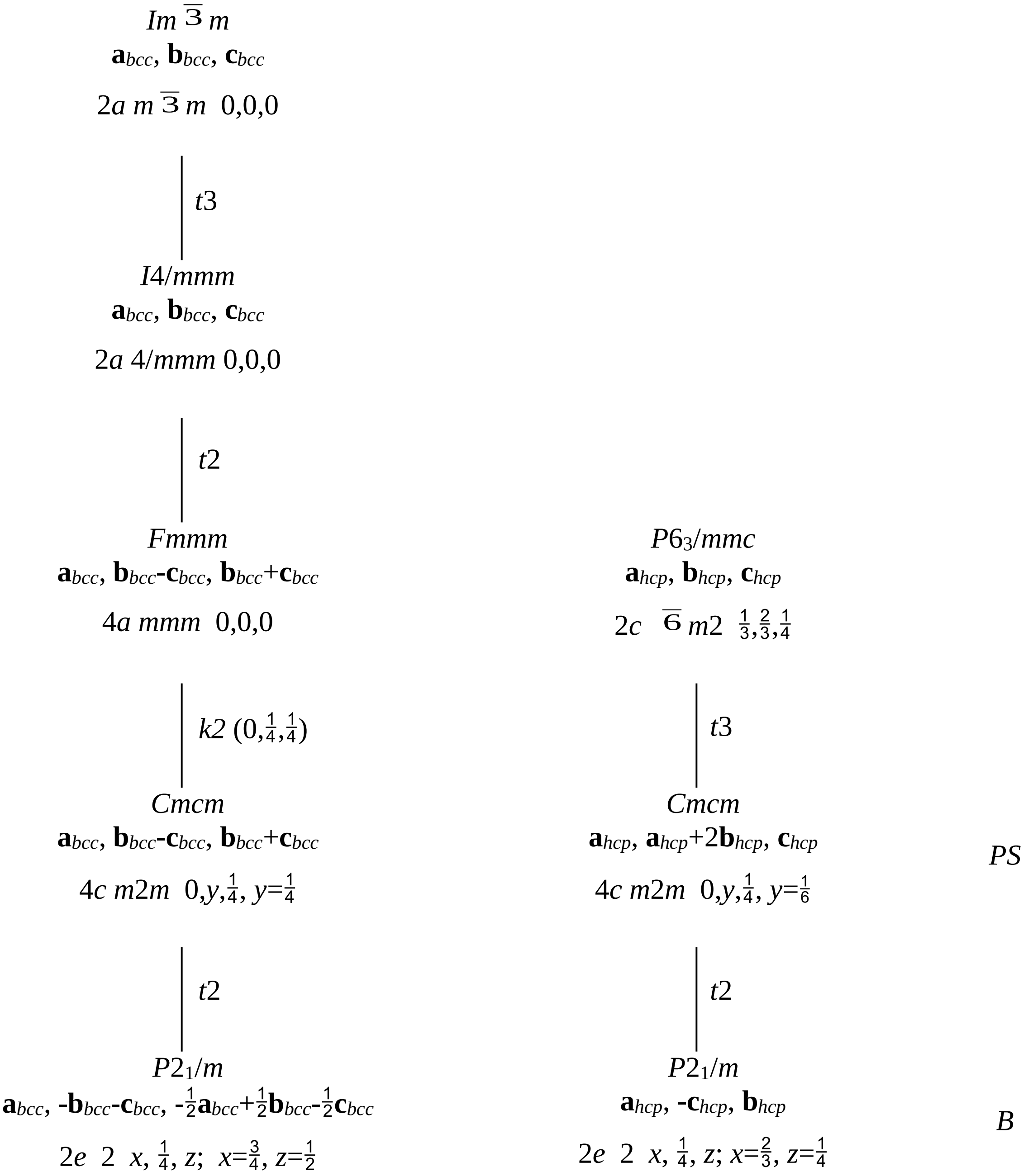

Figure S5 Symmetry relations between *bcc* and *hcp* type structures according to the Pitsch-Schrader (PS) and the Burgers (B) path. The symbols ti or ki indicate translationengleiche or klassengleiche subgroups, respectively. i is the index of the subgroup. The vector specifies the shift of the origin that is necessary to obtain the standard description of the space group.