

Supplementary Materials: Short-Range Stacking Disorder in Mixed-Layer Compounds: a HAADF STEM Study of Bastnäsite-Parisite Intergrowths

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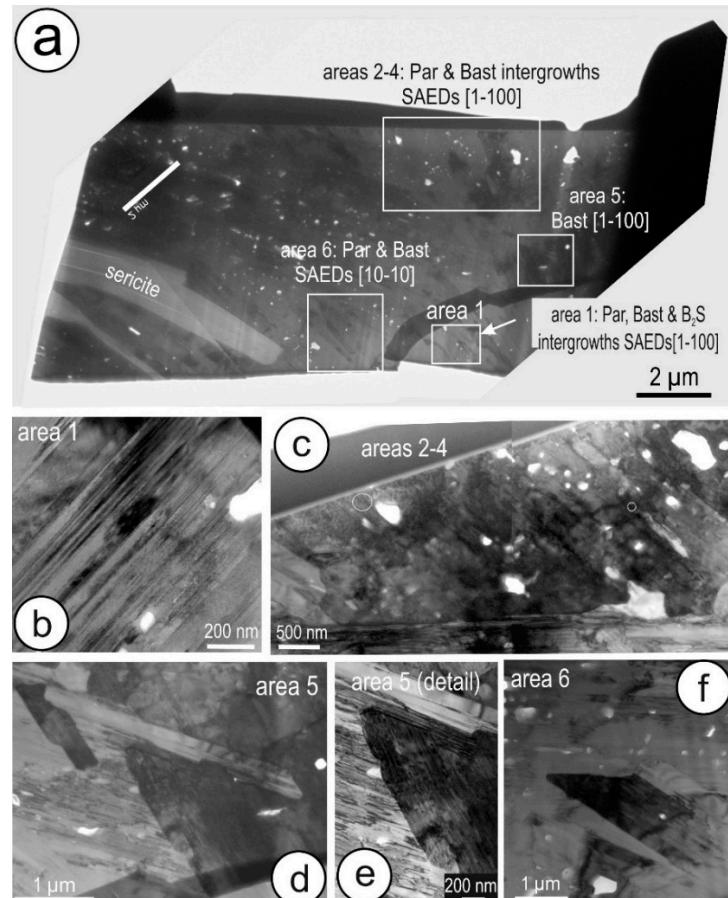


Figure S1. BF TEM images showing Foil 2 (a) and details from areas studied (b–f) showing aspects of the lamellar intergrowths from the two studied foils; (a) Location and main phases in areas 1–6 are shown. The zone axes representing SAEDs from Figures 4 and 5 are also indicated. Note that HAADF STEM imaging for B_2S and associated bastnäsite (Bast) and parisite (Par) from area 1 (e.g., Figure 8c,d) is obtained by tilting the specimen on the $[10 - 10]$ zone axis; (b) Intergrowths with transitional changes in colour from which the B_2S compound was identified; (c) Parisite dominant zone with numerous inclusions of hematite and holes; (d,e) Wedged-shaped bastnasite-dominant domain from which SAEDs typical of disordered bastnäsite were obtained (e.g., Figure 5b). This shows however fine-scale intergrowths of bastnäsite-parisite (Figure 6b), as well as replacement between the two species (Figure 11d).

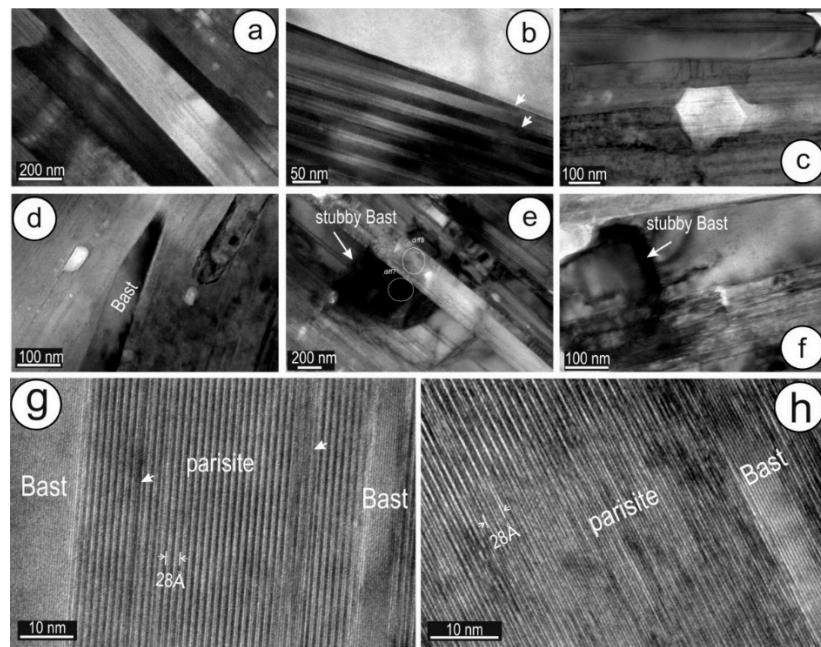


Figure S2. BF TEM images showing aspects of the lamellar intergrowths from the two studied foils: (a) Lamellae of variable colour and widths (hundred to tens of nm) typical of the main part of the syntaxial intergrowths among the BSG minerals; (b) Cuspate termination (arrowed) of thinner lamellae (tens of nm) showing domains of the same dark and grey colour; (c) Parallel, equal-width lamellae with well-shaped edges. Note the hexagonal-shaped, thinner area (from which hematite was plucked-out during milling typical of foil 1) showing the fine-scale layered intergrowths within lamellae of grey colour; (d) Dark lamellae of bastnasite (Bast) cross-cutting layering in other lamellae of lighter colour. Note how the bastnasite tip fades into the other lamellae; (e,f) Stubby bastnasite giving the $c = 2c''$ polytype (Figures 4b and 5b) attributed to 1H bastnäsite; (g,h) HR TEM images showing relatively regular stacking sequences consisting of bastnasite and parisite. Note the presence of defects (arrowed).

Table S1. EPMA data for parisite.

wt %	1	2	3	4	5	6	7	8	9	10	11	12	Mean	SD
CaO	9.33	9.43	8.72	7.15	9.51	8.05	7.29	7.81	7.61	8.37	9.44	9.81	8.54	0.91
K ₂ O	0.03	0.05	0.01	0.03	<mdl	0.06	<mdl	0.02	0.02	0.03	<mdl	<mdl	0.03	0.01
La ₂ O ₃	23.43	23.88	23.96	24.14	24.25	24.68	24.84	24.88	24.98	25.62	26.43	26.66	24.81	0.96
Ce ₂ O ₃	31.46	31.82	33.02	32.79	32.03	32.70	32.70	32.81	33.33	32.90	27.36	27.75	31.72	1.93
F	5.08	4.95	5.72	6.19	4.39	5.64	5.67	5.50	5.88	5.12	4.70	4.45	5.27	0.56
FeO	0.11	0.12	0.81	0.13	<mdl	<mdl	0.26	0.14	0.10	0.30	<mdl	<mdl	0.25	0.23
Tm ₂ O ₃	<mdl	0.06	-											
Gd ₂ O ₃	<mdl	<mdl	0.12	0.17	0.13	<mdl	<mdl	<mdl	0.11	<mdl	0.26	0.26	0.18	0.06
Dy ₂ O ₃	<mdl	<mdl	<mdl	0.05	0.06	<mdl	<mdl	<mdl	<mdl	<mdl	0.12	0.09	0.08	0.02
Tb ₂ O ₃	<mdl	<mdl	<mdl	0.06	<mdl	0.06	-							
Sm ₂ O ₃	0.25	0.21	0.26	0.32	0.29	0.21	0.20	0.21	0.25	0.20	0.28	0.30	0.25	0.04
Eu ₂ O ₃	0.10	0.08	0.07	0.11	0.06	0.10	0.12	0.06	0.08	<mdl	0.13	0.14	0.10	0.02
Nd ₂ O ₃	5.07	4.99	5.06	5.70	5.48	5.17	5.35	5.20	5.35	5.07	5.93	5.84	5.35	0.31
Pr ₂ O ₃	2.15	2.11	2.15	2.47	2.35	2.24	2.21	2.25	2.35	2.29	1.99	1.99	2.21	0.14
SrO	0.03	0.03	0.03	0.04	0.02	0.05	0.03	0.04	0.04	<mdl	0.03	0.05	0.03	0.01
SO ₃	<mdl	<mdl	0.03	0.05	<mdl	0.04	0.01							
Cl	0.08	0.12	0.19	0.07	0.02	0.05	0.03	0.04	0.06	0.05	0.02	0.03	0.06	0.05
ThO ₂	0.11	0.10	0.08	0.06	0.07	0.09	0.05	0.17	0.07	0.12	0.07	0.06	0.09	0.03
Y ₂ O ₃	0.37	0.34	0.30	0.31	0.42	0.30	0.32	0.35	0.31	0.32	0.91	0.83	0.42	0.20
TOTAL	77.93	78.73	80.98	80.26	79.41	79.79	79.49	79.81	81.02	80.78	77.67	78.25	79.51	1.11
O = halogens	-2.16	-2.11	-2.45	-2.75	-1.85	-2.39	-2.39	-2.33	-2.49	-2.17	-1.99	-1.88	-2.25	0.26
CO ₂ (calc.)	19.39	19.51	20.23	19.89	19.46	19.70	19.54	19.64	19.97	19.81	19.33	19.41	19.66	0.26
Total	95.01	95.94	98.63	97.34	96.96	96.86	97.04	98.36	98.28	95.01	95.78	96.81	1.18	
Structural Formulae														
Ca	0.893	0.894	0.816	0.693	0.885	0.771	0.706	0.746	0.724	0.782	0.895	0.917	0.810	0.080
Sr	0.001	0.001	0.001	0.002	0.001	0.002	0.001	0.002	0.002	0.000	0.001	0.002	0.002	0.001
Fe	0.008	0.009	0.059	0.010	0.000	0.000	0.020	0.011	0.007	0.022	0.000	0.000	0.012	0.016
K	0.003	0.006	0.001	0.004	0.000	0.006	0.000	0.002	0.002	0.003	0.000	0.000	0.002	0.002
Total	0.905	0.910	0.877	0.709	0.886	0.780	0.727	0.762	0.736	0.807	0.896	0.920	0.826	0.077
Y	0.018	0.016	0.014	0.015	0.019	0.014	0.015	0.016	0.015	0.015	0.043	0.039	0.020	0.009
La	0.772	0.779	0.771	0.805	0.776	0.814	0.828	0.819	0.818	0.824	0.863	0.858	0.811	0.030
Ce	1.029	1.030	1.055	1.086	1.018	1.070	1.082	1.072	1.083	1.050	0.886	0.887	1.029	0.067
Pr	0.070	0.068	0.068	0.081	0.074	0.073	0.073	0.073	0.076	0.073	0.064	0.063	0.071	0.005
Nd	0.162	0.158	0.158	0.184	0.170	0.165	0.173	0.166	0.170	0.158	0.187	0.182	0.169	0.010
Sm	0.008	0.006	0.008	0.010	0.009	0.006	0.006	0.006	0.008	0.006	0.009	0.009	0.008	0.001
Eu	0.003	0.002	0.002	0.003	0.002	0.003	0.004	0.002	0.002	0.000	0.004	0.004	0.003	0.001
Gd	0.000	0.000	0.004	0.005	0.004	0.000	0.000	0.000	0.003	0.000	0.008	0.007	0.003	0.003
Tb	0.000	0.000	0.000	0.002	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Dy	0.000	0.000	0.000	0.002	0.002	0.000	0.000	0.000	0.000	0.000	0.003	0.002	0.001	0.001
Tm	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.000	0.000	0.000	0.001
Th	0.002	0.002	0.002	0.001	0.001	0.002	0.001	0.003	0.001	0.002	0.001	0.001	0.002	0.001
Total	2.063	2.061	2.082	2.195	2.076	2.148	2.182	2.158	2.176	2.129	2.069	2.053	2.116	0.052
CO ₂	0.000	0.000	0.002	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.001
SO ₃	0.000	0.000	0.002	0.003	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.002	0.001
F	1.436	1.385	1.580	1.770	1.205	1.596	1.620	1.552	1.650	1.411	1.316	1.227	1.479	0.169
Cl	0.013	0.018	0.027	0.011	0.003	0.008	0.005	0.006	0.008	0.007	0.003	0.004	0.009	0.007

Table S2. EPMA data for fluorocarbonates (mixed layer, compositions between bastnäsite and parsite).

wt %	1	2	3	4	5	6	7	8	9	10	11	12	13
CaO	6.45	6.54	5.30	4.56	5.65	3.54	6.54	4.33	3.98	5.26	5.43	5.03	2.55
K ₂ O	<mdl	<mdl	0.01	<mdl	0.03	0.01	0.01	0.03	0.03	0.02	<mdl	<mdl	0.03
La ₂ O ₃	25.55	24.38	24.69	25.09	25.71	26.32	26.56	26.65	26.82	27.25	28.37	29.16	29.68
Ce ₂ O ₃	34.35	32.52	33.25	33.82	34.60	35.62	35.32	35.97	36.41	35.23	37.03	37.32	39.41
F	6.05	6.13	6.37	6.64	5.90	6.73	6.04	6.50	6.50	6.07	6.34	6.22	4.06
FeO	0.41	0.82	0.08	0.33	0.43	0.17	0.39	0.61	0.46	<mdl	0.39	<mdl	0.20
Tm ₂ O ₃	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl
Gd ₂ O ₃	0.12	<mdl	0.10	<mdl	0.15	0.16	0.11	<mdl	0.14	<mdl	0.13	<mdl	0.17
Dy ₂ O ₃	<mdl	<mdl	<mdl	<mdl	<mdl	0.06	0.06	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl
Tb ₂ O ₃	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	<mdl	0.04	<mdl	<mdl	<mdl	<mdl	<mdl
Sm ₂ O ₃	0.28	0.20	0.25	0.28	0.34	0.32	0.28	0.27	0.33	0.17	0.26	0.18	0.16
Eu ₂ O ₃	0.11	0.08	0.12	0.11	0.14	0.13	0.10	0.10	0.11	0.09	0.11	0.07	0.08
Nd ₂ O ₃	5.66	5.21	5.51	5.53	5.55	5.48	5.47	5.90	5.76	5.13	5.76	5.42	5.31
Pr ₂ O ₃	2.36	2.20	2.31	2.38	2.39	2.27	2.32	2.61	2.53	2.28	2.54	2.55	2.24
SrO	<mdl	0.03	0.04	0.05	0.04	0.02	0.02	0.03	0.05	0.03	0.02	0.04	0.04
SO ₃	<mdl	<mdl	<mdl	<mdl	0.03	<mdl	<mdl	0.04	0.03	<mdl	<mdl	<mdl	<mdl
Cl	0.05	0.12	0.02	0.04	0.10	0.04	0.07	0.03	0.03	0.02	0.03	0.03	0.02
ThO ₂	0.04	0.05	0.07	0.07	0.16	0.08	0.08	0.06	0.08	0.03	0.10	0.05	0.12
Y ₂ O ₃	0.32	0.33	0.32	0.38	0.32	0.36	0.34	0.33	0.33	0.31	0.34	0.32	0.35
Total	82.26	79.09	79.09	79.81	81.55	81.29	83.72	83.48	83.59	81.88	86.82	86.39	84.42
O = halogens	-2.56	-2.61	-2.69	-2.80	-2.51	-2.84	-2.56	-2.75	-2.74	-2.56	-2.68	-2.62	-1.72
CO ₂ (calc.)	20.09	19.55	19.31	19.45	20.81	20.19	20.50	20.26	20.18	19.85	21.03	20.77	19.11
Total	99.61	95.85	95.60	96.31	100.38	102.63	102.01	101.43	101.42	99.50	105.18	104.54	102.15
Structural Formulae													
Ca	0.613	0.645	0.536	0.461	0.514	0.353	0.607	0.415	0.382	0.507	0.493	0.461	0.239
Sr	0.000	0.001	0.002	0.003	0.002	0.001	0.001	0.002	0.003	0.002	0.001	0.002	0.002
Fe	0.030	0.063	0.006	0.026	0.244	0.013	0.028	0.046	0.035	0.000	0.028	0.000	0.015
K	0.000	0.000	0.002	0.000	0.003	0.001	0.001	0.003	0.004	0.002	0.000	0.000	0.003
Total	0.643	0.710	0.546	0.489	0.763	0.368	0.637	0.465	0.423	0.510	0.521	0.463	0.259
Y	0.015	0.016	0.016	0.019	0.015	0.018	0.016	0.015	0.016	0.015	0.015	0.015	0.017
La	0.836	0.827	0.858	0.872	0.805	0.905	0.847	0.878	0.887	0.904	0.886	0.920	0.960
Ce	1.115	1.095	1.147	1.167	1.075	1.216	1.119	1.177	1.196	1.160	1.148	1.169	1.265
Pr	0.076	0.074	0.079	0.082	0.074	0.077	0.073	0.085	0.083	0.075	0.078	0.080	0.071
Nd	0.179	0.171	0.186	0.186	0.168	0.182	0.169	0.188	0.185	0.165	0.174	0.166	0.166
Sm	0.009	0.006	0.008	0.009	0.010	0.010	0.008	0.008	0.010	0.005	0.008	0.005	0.005
Eu	0.003	0.002	0.004	0.003	0.004	0.004	0.003	0.003	0.003	0.003	0.003	0.002	0.002
Gd	0.004	0.000	0.003	0.000	0.004	0.005	0.003	0.000	0.004	0.000	0.004	0.000	0.005
Tb	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.001	0.000	0.000	0.000	0.000	0.000
Dy	0.000	0.000	0.000	0.000	0.000	0.002	0.002	0.000	0.000	0.000	0.000	0.000	0.000
Tm	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Th	0.001	0.001	0.001	0.002	0.003	0.002	0.002	0.001	0.002	0.001	0.002	0.001	0.002
Total	2.238	2.193	2.303	2.340	2.158	2.421	2.242	2.357	2.385	2.327	2.318	2.358	2.494
CO ₂													
SO ₃	0.000	0.000	0.000	0.000	0.002	0.000	0.000	0.003	0.002	0.000	0.000	0.000	0.000
F	1.697	1.784	1.899	1.979	1.583	1.986	1.652	1.838	1.844	1.727	1.699	1.683	1.127
Cl	0.008	0.019	0.004	0.006	0.015	0.006	0.011	0.004	0.004	0.003	0.005	0.004	0.003

Table S3. EPMA data for bastnäsite.

wt %	1	2	3	4	5	6	7	Mean	SD
CaO	0.35	0.07	0.07	0.16	0.05	0.27	0.40	0.20	0.13
K ₂ O	0.01	0.04	0.01	<mdl	0.01	0.05	0.03	0.03	0.02
La ₂ O ₃	27.05	27.11	27.19	27.23	28.28	29.35	30.33	28.08	1.21
Ce ₂ O ₃	36.18	34.93	34.85	35.97	35.69	38.83	39.59	36.58	1.74
F	7.18	6.97	7.39	7.14	7.08	5.83	6.39	6.85	0.51
FeO	0.14	0.18	<mdl	0.06	<mdl	0.24	0.09	0.14	0.07
Tm ₂ O ₃	<mdl	-	-						
Gd ₂ O ₃	0.16	<mdl	<mdl	<mdl	<mdl	0.13	<mdl	0.15	0.02
Dy ₂ O ₃	<mdl	-	-						
Tb ₂ O ₃	<mdl	-	-						
Sm ₂ O ₃	0.26	0.29	0.26	0.18	0.25	0.24	0.32	0.26	0.04
Eu ₂ O ₃	0.09	0.13	0.09	0.08	0.11	0.13	0.13	0.11	0.02
Nd ₂ O ₃	6.08	5.90	5.69	4.95	5.39	5.76	6.28	5.72	0.41
Pr ₂ O ₃	2.65	2.50	2.51	2.24	2.36	2.45	2.77	2.50	0.16
SrO	0.04	0.03	0.05	0.04	0.03	0.02	0.03	0.04	0.01
SO ₃	0.03	<mdl	2.78	0.11	0.55	0.04	<mdl	0.70	1.06
Cl	0.03	0.01	0.03	0.01	0.03	0.02	0.03	0.02	0.01
ThO ₂	0.19	0.16	0.08	0.15	0.10	0.18	0.16	0.14	0.04
Y ₂ O ₃	0.27	0.21	0.14	0.27	0.34	0.31	0.31	0.26	0.06
Total	80.71	78.54	81.13	78.58	80.27	83.84	86.85	81.42	2.77
O = halogens	-3.03	-2.94	-3.12	-3.01	-2.99	-2.46	-2.70	-2.89	0.21
CO ₂ (calc.)	19.16	18.57	20.94	18.66	19.25	19.27	20.07	19.42	0.77
Total	97.49	94.82	99.46	94.37	96.79	101.15	104.72	98.40	3.41
Structural Formulae									
Ca	0.037	0.008	0.007	0.017	0.005	0.027	0.039	0.020	0.013
Sr	0.002	0.002	0.003	0.002	0.002	0.001	0.002	0.002	0.001
Fe	0.012	0.015	0.000	0.005	0.000	0.019	0.006	0.008	0.007
K	0.001	0.005	0.002	0.000	0.001	0.006	0.003	0.003	0.002
Total	0.052	0.030	0.012	0.024	0.009	0.052	0.050	0.033	0.017
Y	0.014	0.011	0.008	0.014	0.018	0.015	0.015	0.014	0.003
La	0.983	1.014	1.027	1.021	1.043	1.005	1.006	1.014	0.018
Ce	1.304	1.297	1.307	1.339	1.306	1.319	1.303	1.311	0.013
Pr	0.095	0.093	0.094	0.083	0.086	0.083	0.091	0.089	0.005
Nd	0.214	0.214	0.208	0.180	0.192	0.191	0.202	0.200	0.012
Sm	0.009	0.010	0.009	0.006	0.009	0.008	0.010	0.009	0.001
Eu	0.003	0.005	0.003	0.003	0.004	0.004	0.004	0.004	0.001
Gd	0.005	0.000	0.000	0.000	0.000	0.004	0.000	0.001	0.002
Tb	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Dy	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Tm	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000	0.000
Th	0.004	0.004	0.002	0.003	0.002	0.004	0.003	0.003	0.001
Total	2.631	2.647	2.659	2.649	2.660	2.633	2.633	2.645	0.012
CO ₂									
SO ₃	0.002	0.000	0.214	0.008	0.041	0.003	0.000	0.037	0.000
F	2.235	2.236	2.393	2.297	2.238	1.711	1.817	2.122	0.000
Cl	0.005	0.001	0.004	0.001	0.004	0.004	0.005	0.004	0.000

Table S4. (A) Parasite and (B) unnamed B2S polytypes.

Polytype	c''' (Å)	$x n_1$	c' (Å)	$x n_2$	c (Å)
(A)					
3R *	4.71			3	14
6R *	4.71			6	28
6R1	4.71	6	28	18	85
6R2	4.71			18	85
18R	4.71	18	85	54	254
24R	4.71	24	113	72	339
30R	4.71	30	141	90	424
36R	4.71	36	170	108	509
42R	4.71	42	198	126	593
2H **	4.71			6	28
8H	4.71			24	113
10H	4.71			30	141
14H	4.71			42	198
16H	4.71			48	226
(B)					
6R	4.8	8	38	24	115
12R	4.8	16	77	48	230
24R	4.8	32	154	96	461
2H1	4.8			8	38
2H2 **	4.8			8	38
4H	4.8			16	77
12H	4.8			48	230

Note: after Meng et al. [19,21,22]; * after Van Landuyt and Amelinckx (1975) [16]; ** polytypes present in this study; R—rhombohedral; H—hexagonal.