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MATERIALS

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Supporting information for article:

Jinshajiangite: structure, twinning and pseudosymmetry

Shiyun Jin, Huifang Xu, Seungyeol Lee and Pingqiu Fu

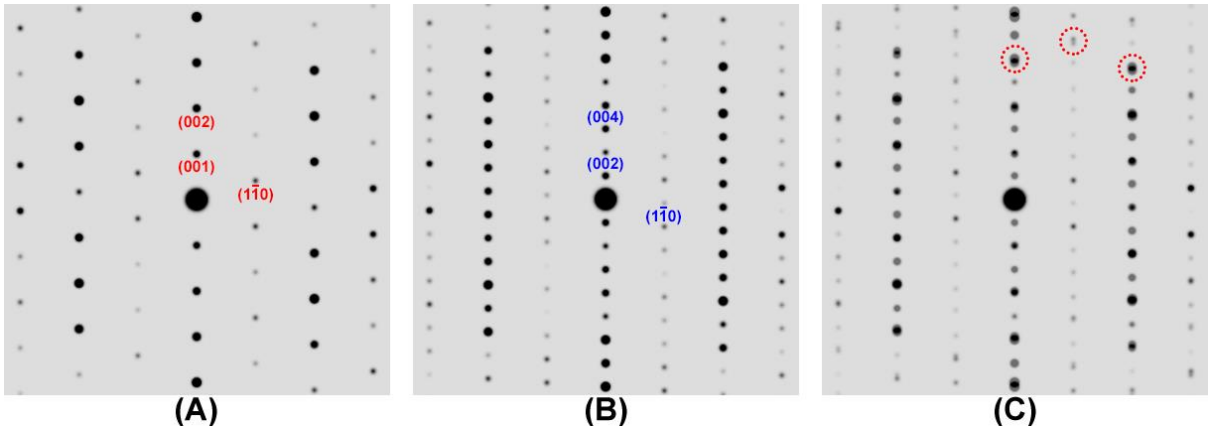

Figure S1 Simulated [110] zone axis diffraction pattern of (A) bafertisite type-I, (B) camaraite, and (C) intergrown bafertisite and camaraite.

S1. Polytype structure of bafertisite.

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#======================================================================

# CRYSTAL DATA

#----------------------------------------------------------------------

data_bafertisite_1Tc1


_pd_phase_name                      'bafertisite'
_cell_length_a                     10.6770(54)
_cell_length_b                     13.7670(41)
_cell_length_c                     11.737(5)
_cell_angle_alpha                   90.11(2)
_cell_angle_beta                   112.280(32)
_cell_angle_gamma                   90.020(45)
_symmetry_space_group_name_H-M        'C -1'
_symmetry_Int_Tables_number           2

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_symmetry_equiv_pos_as_xyz
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  '-x, -y, -z'
  'x+1/2, y+1/2, z'
  '-x+1/2, -y+1/2, -z'

loop_
  _atom_site_label
  _atom_site_occupancy
  _atom_site_fract_x
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  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  AP1      1.0    0.61159(3)    0.62480(3)    0.468362(16) Uiso  0.008952 Ba
  AP2      1.0    0.38933(3)    0.87896(3)    0.535339(19) Uiso  0.017492 Ba
  MH1      1.0    0.46521(6)    0.60392(6)    0.71645(6)   Uiso  0.005187 Ti
  MH2      1.0    0.53602(6)    0.85602(6)    0.28617(5)   Uiso  0.004961 Ti
  MO1      1.0    0.000000      0.000000      0.000000     Uiso  0.008945 Fe
  MO2      1.0    0.500000      0.000000      0.000000     Uiso  0.014673 Fe
  MO3      1.0    0.24428(5)    0.12334(5)    0.98780(4)   Uiso  0.008359 Fe
  MO4      1.0    0.25574(5)    0.87305(5)    0.00842(4)   Uiso  0.008188 Fe
  MO5      1.0    0.49526(5)    0.25210(5)    0.99381(5)   Uiso  0.010044 Fe
  Si1      1.0    0.28268(10)   0.01517(10)   0.24709(10)  Uiso  0.005600 Si
  Si2      1.0    0.24186(10)   0.98299(10)   0.75141(10)  Uiso  0.005479 Si
  Si3      1.0    0.71702(10)   0.76397(10)   0.75114(10)  Uiso  0.005703 Si
  Si4      1.0    0.75880(10)   0.23729(10)   0.24802(10)  Uiso  0.005826 Si
  XH11     1.0    0.1698(4)     0.0012(4)     0.3056(4)    Uiso  0.011890 O
  XH12     1.0    0.0813(4)     0.9992(4)     0.6953(4)    Uiso  0.011113 O
  XH13     1.0    0.5825(4)     0.6987(4)     0.6828(2)    Uiso  0.011128 O
  XH14     1.0    0.3165(4)     0.6964(4)     0.6819(4)    Uiso  0.010849 O
  XH21     1.0    0.4165(4)     0.9509(4)     0.3206(4)    Uiso  0.010888 O
  XH22     1.0    0.3190(4)     0.0479(4)     0.6833(4)    Uiso  0.010658 O
  XH23     1.0    0.6715(4)     0.7524(4)     0.3084(4)    Uiso  0.010893 O
  XH24     1.0    0.4198(4)     0.7521(4)     0.3108(4)    Uiso  0.010588 O
  XOA1     1.0    0.4559(4)     0.6242(4)     0.0848(2)    Uiso  0.009326 O
  XOA2     1.0    0.4533(4)     0.1278(4)     0.0770(2)    Uiso  0.008789 O
  XOM1     1.0    0.5368(4)     0.6160(4)     0.8821(2)    Uiso  0.009509 O
  XOM2     1.0    0.4637(4)     0.8660(4)     0.1220(2)    Uiso  0.010416 O
  XOSi1    1.0    0.2175(4)     0.9999(4)     0.0986(4)    Uiso  0.008096 O
  XOSi2    1.0    0.2983(4)     0.9960(4)     0.9008(4)    Uiso  0.007304 O
  XOSi3    1.0    0.2847(4)     0.2509(4)     0.9001(4)    Uiso  0.008392 O
  XOSi4    1.0    0.7040(4)     0.2505(4)     0.0986(4)    Uiso  0.008063 O
  XPM1     1.0    0.1176(4)     0.9062(4)     0.4769(2)    Uiso  0.015144 F
  XPM2     1.0    0.6147(4)     0.8524(4)     0.4797(2)    Uiso  0.018091 F
  Xsi1     1.0    0.6548(4)     0.8746(4)     0.7252(2)    Uiso  0.009135 O
  Xsi2     1.0    0.2802(4)     0.8726(4)     0.7230(2)    Uiso  0.009277 O

loop_
  _atom_site_aniso_label
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_12
  _atom_site_aniso_U_13
  _atom_site_aniso_U_23
  AP1    0.00763  0.01099  0.00860 -0.00062  0.00349 -0.00037
  AP2    0.00896  0.03346  0.01079 -0.00237  0.00458 -0.00081
  MH1    0.00310  0.00760  0.00530 -0.00066  0.00209 -0.00023
  MH2    0.00290  0.00730  0.00530 -0.00042  0.00225  0.00013
  MO1    0.00670  0.00810  0.01260 -0.00030  0.00430 -0.00050
  MO2    0.00550  0.01620  0.01950  0.00050  0.00160 -0.00880
  MO3    0.00629  0.00860  0.01060 -0.00110  0.00367  0.00000
  MO4    0.00680  0.00790  0.01050 -0.00111  0.00400 -0.00060
  MO5    0.00610  0.00961  0.01420 -0.00140  0.00359  0.00170
  Si1    0.00530  0.00520  0.00660 -0.00110  0.00260 -0.00080
  Si2    0.00490  0.00510  0.00670 -0.00150  0.00250 -0.00060
  Si3    0.00510  0.00610  0.00630 -0.00140  0.00260  0.00050
  Si4    0.00540  0.00580  0.00680  0.00020  0.00290  0.00041
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  XH11  0.00970  0.01369  0.01570 -0.00480  0.00870 -0.00401
  XH12  0.00580  0.01250  0.01430 -0.00070  0.00300 -0.00470
  XH13  0.00920  0.01401  0.01140 -0.00460  0.00530 -0.00110
  XH14  0.01071  0.01020  0.01320  0.00240  0.00630 -0.00120
  XH21  0.00880  0.01220  0.01260  0.00360  0.00510  0.00260
  XH22  0.00800  0.01209  0.01130 -0.00450  0.00300  0.00000
  XH23  0.01030  0.01050  0.01530  0.00160  0.00870  0.00320
  XH24  0.00650  0.01101  0.01310 -0.00140  0.00240  0.00240
  XOA1  0.00900  0.01070  0.00800  0.00100  0.00290  0.00130
  XOA2  0.00790  0.00939  0.00930  0.00180  0.00350  0.00240
  XOM1 0.00790  0.01320  0.00810 -0.00260  0.00380 -0.00090
  XOM2 0.00700  0.01539  0.00960 -0.00130  0.00400 -0.00290
  XOSi1 0.00790  0.00990  0.00540 -0.00200  0.00130 -0.00090
  XOSi2 0.00590  0.01001  0.00520  0.00010  0.00120 -0.00061
  XOSi3 0.00760  0.01161  0.00660  0.00030  0.00340  0.00170
  XOSi4 0.00760  0.01029  0.00620 -0.00080  0.00250  0.00120
  XPM1  0.01020  0.02761  0.00680 -0.00130  0.00230 -0.00040
  XPM2  0.00970  0.03610  0.00760 -0.00090  0.00230 -0.00100
  Xsi1    0.00870  0.00780  0.01150  0.00100  0.00450  0.00030
  Xsi2    0.01030  0.00780  0.01110  0.00030  0.00560  0.00030
#=============================================================================

# CRYSTAL DATA

#------------------------------------------------------------------------

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_pd_phase_name                      'bafertisite'
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_cell_length_b                     13.7670(41)
_cell_length_c                     10.90(3)
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_cell_angle_beta                    85.33(13)
_cell_angle_gamma                     90.020(45)
_symmetry_space_group_name_H-M         'C -1'
_symmetry_Int_Tables_number           2

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_symmetry_equiv_pos_as_xyz
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  'x+1/2, y+1/2, z'
  '-x+1/2, -y+1/2, -z'

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  _atom_site_occupancy
  _atom_site_fract_x
  _atom_site_fract_y
  _atom_site_fract_z
  _atom_site_adp_type
  _atom_site_U_iso_or_equiv
  _atom_site_type_symbol
  AP1       1.0     0.87741(6)    0.12480(5)    0.468362(16) Uiso  0.008964 Ba
  AP2       1.0     0.37834(6)    0.12104(5)    0.464661(19) Uiso  0.017494 Ba
  MH1       1.0     0.89302(14)   0.89608(12)   0.28355(6)   Uiso  0.005186 Ti
  MH2       1.0     0.39294(12)   0.85601(10)   0.28617(5)   Uiso  0.004958 Ti
  MO1       1.0     0.000000      0.000000      0.000000     Uiso  0.008936 Fe
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  MO2      1.0    0.500000     0.000000     0.000000    Uiso  0.014672 Fe
  MO3      1.0    0.74962(10)  0.87666(9)   0.01220(4)  Uiso  0.008360 Fe
  MO4      1.0    0.25153(10)  0.87305(9)   0.00842(4)  Uiso  0.008183 Fe
  MO5      1.0    0.00165(12)  0.24790(10)  0.00619(5)  Uiso  0.010046 Fe
  Si1      1.0    0.1591(4)    0.0152(4)    0.24709(10) Uiso  0.005609 Si
  Si2      1.0    0.6338(4)    0.0170(4)    0.24859(10) Uiso  0.005487 Si
  Si3      1.0    0.6585(4)    0.7361(4)    0.24886(10) Uiso  0.005708 Si
  Si4      1.0    0.6348(4)    0.2373(4)    0.24802(10) Uiso  0.005820 Si
  XH11     1.0    0.0170(9)    0.0012(8)    0.3056(4)   Uiso  0.011885 O
  XH12     1.0    0.7663(9)    0.0008(8)    0.3047(4)   Uiso  0.011107 O
  XH13     1.0    0.7589(7)    0.8013(7)    0.3172(2)   Uiso  0.011131 O
  XH14     1.0    0.5245(9)    0.3036(8)    0.3181(4)   Uiso  0.010841 O
  XH21     1.0    0.2562(9)    0.9509(8)    0.3206(4)   Uiso  0.010889 O
  XH22     1.0    0.5227(9)    0.9521(8)    0.3167(4)   Uiso  0.010647 O
  XH23     1.0    0.5173(9)    0.7524(8)    0.3084(4)   Uiso  0.010887 O
  XH24     1.0    0.7644(9)    0.2521(8)    0.3108(4)   Uiso  0.010589 O
  XOA1     1.0    0.9135(7)    0.1242(7)    0.0848(2)   Uiso  0.009333 O
  XOA2     1.0    0.9148(7)    0.6278(7)    0.0770(2)   Uiso  0.008796 O
  XOM1     1.0    0.9043(7)    0.8840(7)    0.1179(2)   Uiso  0.009512 O
  XOM2     1.0    0.9027(7)    0.3660(7)    0.1220(2)   Uiso  0.010421 O
  XOSi1    1.0    0.6653(9)    0.7491(8)    0.0999(4)   Uiso  0.008388 O
  XOSi2    1.0    0.6521(9)    0.0040(8)    0.0992(4)   Uiso  0.007302 O
  XOSi3    1.0    0.1682(9)    0.9999(8)    0.0986(4)   Uiso  0.008102 O
  XOSi4    1.0    0.6547(9)    0.2505(8)    0.0986(4)   Uiso  0.008071 O
  XPM1     1.0    0.8791(7)    0.9062(7)    0.4769(2)   Uiso  0.015144 F
  XPM2     1.0    0.3749(7)    0.8523(7)    0.4797(2)   Uiso  0.018094 F
  Xsi1     1.0    0.7078(7)    0.6254(7)    0.2748(2)   Uiso  0.009133 O
  Xsi2     1.0    0.5813(7)    0.1274(7)    0.2770(2)   Uiso  0.009273 O

loop_
  _atom_site_aniso_label
  _atom_site_aniso_U_11
  _atom_site_aniso_U_22
  _atom_site_aniso_U_33
  _atom_site_aniso_U_12
  _atom_site_aniso_U_13
  _atom_site_aniso_U_23
  AP1   0.00724  0.01102  0.00860 -0.00049 -0.00046 -0.00036
  AP2   0.00815  0.03347  0.01079 -0.00216 -0.00035 -0.00081
  MH1   0.00267  0.00759  0.00530 -0.00060 -0.00035 -0.00024
  MH2   0.00226  0.00729  0.00530 -0.00052 -0.00017  0.00013
  MO1   0.00624  0.00809  0.01260 -0.00007 -0.00153 -0.00052
  MO2   0.00938  0.01620  0.01950  0.00485 -0.00784 -0.00880
  MO3   0.00598  0.00859  0.01060 -0.00118 -0.00124  0.00000
  MO4   0.00618  0.00789  0.01050 -0.00089 -0.00083 -0.00061
  MO5   0.00671  0.00960  0.01420 -0.00234 -0.00309  0.00170
  Si1   0.00501  0.00521  0.00660 -0.00080 -0.00044 -0.00081
  Si2   0.00467  0.00511  0.00670 -0.00132 -0.00059 -0.00060
  Si3   0.00470  0.00610  0.00630 -0.00175 -0.00030  0.00051
  Si4   0.00483  0.00579  0.00680  0.00002 -0.00021  0.00040
  XH11  0.00582  0.01370  0.01570 -0.00321  0.00168 -0.00401
  XH12  0.00699  0.01249  0.01430  0.00155 -0.00377 -0.00469
  XH13  0.00783  0.01401  0.01140 -0.00441  0.00011 -0.00110
  XH14  0.00893  0.01019  0.01320  0.00317  0.00032 -0.00119
  XH21  0.00784  0.01221  0.01260  0.00261 -0.00067  0.00261
  XH22  0.00881  0.01207  0.01130 -0.00484 -0.00230  0.00000
  XH23  0.00642  0.01050  0.01530  0.00016  0.00189  0.00319
  XH24  0.00817  0.01099  0.01310 -0.00267 -0.00383  0.00240
  XOA1  0.00931  0.01071  0.00800  0.00043 -0.00081  0.00130
  XOA2  0.00771  0.00940  0.00930  0.00076 -0.00078  0.00240
```

XOM1	0.00710	0.01321	0.00810	-0.00235	0.00013	-0.00090
XOM2	0.00620	0.01541	0.00960	0.00001	-0.00039	-0.00289
XOSi1	0.00681	0.01160	0.00660	-0.00050	0.00043	0.00170
XOSi2	0.00683	0.01000	0.00520	0.00041	-0.00126	-0.00061
XOSi3	0.00910	0.00991	0.00540	-0.00171	-0.00125	-0.00090
XOSi4	0.00767	0.01031	0.00620	-0.00146	-0.00035	0.00120
XPM1	0.01104	0.02761	0.00680	-0.00121	-0.00085	-0.00039
XPM2	0.01065	0.03611	0.00760	-0.00048	-0.00125	-0.00100
Xsi1	0.00809	0.00781	0.01150	0.00093	-0.00079	0.00030
Xsi2	0.00870	0.00779	0.01110	0.00019	0.00060	0.00029