

Supporting Information

Structures, influences and formation mechanism of planar defects on (100), (001) and (-201) planes in β -Ga₂O₃ crystals

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Table S1 The lattice constants, number of atoms, sectional areas A, and chosen k-point meshes of the different type of TB and SF supercells with lowest energy.

	Lattice constants / Å	Number of atoms	Sectional areas / Å ²	K-point meshes
(100)-twin	a=24.8, b=3.1, c=5.9	40	18.2	1 × 8 × 4
(001)-twin	a=11.9, b=3.0, c=11.9	40	35.9	2 × 8 × 2
(-201)-twin	a=14.8, b=3.1, c=24.0	80	45.5	2 × 8 × 1
(100)-SF	a=48.5, b=3.1, c=5.9	80	18.4	1 × 8 × 4
(001)-SF	a=12.3, b=3.1, c=14.7	50	37.6	2 × 8 × 2
(-201)-SF	a=14.8, b=3.1, c=21.4	70	45.9	2 × 8 × 1

The supercell structure with the lowest energy among each type of TBs and SFs is provided in the format of VASP POSCAR:

1. (100)-twin A

```
(100)twin A
  1.000000000000000
  24.8243170083357292  0.000000000000000  0.0228692036324418
  0.000000000000000  3.0851922584475568  0.000000000000000
  -1.4031753291568423  0.000000000000000  5.7206929828013751
Ga  O
  16  24
Direct
  0.0460024252296665 -0.000000000000000  0.7998730583390160
  0.4544975201323013 -0.000000000000000  0.2081556268162630
  0.2959153124443955  0.500000000000000  0.2974456967593976
  0.1704778933453332 -0.000000000000000  0.1621095966523232
  0.0800065850363250  0.500000000000000  0.3504848552860686
  0.4204663876327736  0.500000000000000  0.6575686825369303
  0.3299864841456890 -0.000000000000000  0.8461309412467412
  0.2045383656189732  0.500000000000000  0.7108045671140553
  0.9544818833952942 -0.000000000000000  0.2077713734922328
  0.7959701296841123  0.500000000000000  0.8013314512739664
  0.7045764524512524  0.500000000000000  0.2051321908485884
  0.5800453438804526  0.500000000000000  0.3164250349115698
  0.9204619267705364  0.500000000000000  0.6903218935531028
  0.8300160344031903  0.000000000000000  0.3207388854671656
  0.6705359005822169 -0.000000000000000  0.6857285874913422
  0.5460228587203588 -0.000000000000000  0.7989950500743837
  0.0863405473846155 -0.000000000000000  0.1185372280475994
  0.4141341837465090 -0.000000000000000  0.8895131777719281
  0.3342462307400625  0.500000000000000  0.0592972074698359
  0.1662043427583500  0.500000000000000  0.9489265293001699
  0.0849994068331084 -0.000000000000000  0.5640426578097364
  0.4154802158005610 -0.000000000000000  0.4439499656311614
  0.3366760559108872  0.500000000000000  0.6157321804347818
  0.1637954902762299  0.500000000000000  0.3924866394224990
  0.4986180456741764  0.500000000000000  0.2490050501078979
  0.0018870333488716  0.500000000000000  0.7585451706681409
  0.2518946992706859 -0.000000000000000  0.2622319991810235
  0.2485635257112753 -0.000000000000000  0.7460746441253862
  0.5850426451163855 -0.000000000000000  0.1128577486598159
  0.9154461633451583 -0.000000000000000  0.8939232862603271
  0.8343043346128650  0.500000000000000  0.1161295849247771
  0.6662600366033048  0.500000000000000  0.8903243083715306
  0.5863873168241749 -0.000000000000000  0.5610652110555365
  0.9141445747751827 -0.000000000000000  0.4457493938442407
  0.8366869675581509  0.500000000000000  0.5644639108863435
  0.6638443106585318  0.500000000000000  0.4419777912569429
  0.9985806250884940  0.500000000000000  0.2550916431956690
  0.5019136558587245  0.500000000000000  0.7521940842936865
  0.7485979055783726 -0.000000000000000  0.2578470548416812
  0.7519501760524455 -0.000000000000000  0.7483961025761379
```

2. (001)-twin A

```
(001)twin A
  1.000000000000000
  11.8972204261877437  0.0431052792284225  0.0299463475721164
  0.0107217870946489  3.0169726329344018  0.0137730950731528
  -2.6730654179367681  0.0429571757215096  11.6306119732467668
Ga  O
  16  24
Direct
  0.1084125269526454  0.9719432375593693  0.4128098608304431
  0.0660129553875448  0.0657115220505283  0.1407643110265831
```

0.6596205450497228	0.9827361035368188	0.4262644144211479
0.5215474554975025	0.4823227901228924	0.2246927149317913
0.8096280042145423	0.9098991455719851	0.0841377604707690
0.3355337740063278	0.9953966669357277	0.3283656846416690
0.3351776090365617	0.9892129694322239	0.0754054531683229
0.9156493288671502	0.9825228487898130	0.6038563468912220
0.8492792239714174	0.4862646639369776	0.3378857500936866
0.0918704778937311	0.9438783498810499	0.8911061966200269
0.6079833466438813	0.4529677624394293	0.9147032437710034
0.3956232253492825	0.4848862983768342	0.5849089475341364
0.1733055238794232	0.4734689996006198	0.6645893704043422
0.8353833361395241	0.4664196092236113	0.8328343588386159
0.6507729428281052	0.9739997602924166	0.6613642701294500
0.3532920361884965	0.9704536769873765	0.8414677043991644
0.7055106430656489	0.4265116868080600	0.0610344095080855
0.3211012703879347	0.4919682267678112	0.4295638664366115
0.1697722766813933	0.9988514774647399	0.0422899789567883
0.8318335883342337	0.9816386178170387	0.4531945753296142
0.0158027041639201	0.4756658605688110	0.4047751978482365
0.3419104066385200	0.4874647815335677	0.1990790325435723
0.5007481282331020	0.9854001098095054	0.3420354032522783
0.861099522638509	0.9902162583444255	0.2419955428624138
0.9712516079986515	0.5659770484426011	0.1036230947591045
0.1679617986213927	0.9919593714434991	0.2813666234896181
0.5013303680599154	0.9842307755768946	0.1198297458545496
0.6778464215732976	0.4860869468563049	0.3196566344530493
0.1986174627963140	0.9752175888087017	0.5649732992499522
0.8157756899673232	0.9641313983559495	0.9269538159073175
0.6633393050236552	0.4790003324926525	0.5448149031297608
0.3311329681926912	0.4796072957813087	0.9524269162241491
0.1813905675839497	0.9703044139393177	0.7800974185911037
0.8237101243476301	0.9703499492915728	0.7126793694366957
0.6610419433029754	0.4697350495384203	0.7716546919170880
0.3444699049142682	0.4715435221455061	0.7277336069126887
0.0080421828331776	0.4789726910807240	0.6332371935621639
0.0003587612880332	0.4496502295821904	0.8633199017342091
0.4877585065221967	0.9811626686649143	0.6077507075233599
0.5166012003000943	0.9574292831478011	0.8853676313452090

3. (-201)-twin A

(-201)twin A

1.0000000000000000		
14.7969927929548355	0.0000000000000000	0.2454274350099350
0.0000000000000000	3.0726568240606373	0.0000000000000000
14.4696306041946183	0.0000000000000000	19.1551689839524961

Ga O
32 48

Direct

0.6132697805260490	0.5000000000000000	0.6605675407783701
0.3084833179085092	0.0000000000000000	0.2604839260831716
0.6742838867676498	0.0000000000000000	0.7604527541754268
0.1132657860521732	0.0000000000000000	0.6605705483827583
0.9142136817231634	0.0000000000000000	0.8574152916028583
0.1742855966866315	0.5000000000000000	0.7604523416945336
0.4142117067432841	0.5000000000000000	0.8574165125297079
0.5974903947254091	0.5000000000000000	0.9129913024155822
0.8578985828196536	0.5000000000000000	0.7574640700044047
0.0974896810912925	0.0000000000000000	0.9129908414634590
0.3579029896142563	0.0000000000000000	0.7574619404391839
0.8916353754359044	0.0000000000000000	0.1186756008904958
0.3413373302442936	0.0000000000000000	0.0129717827965953
0.3916352744976181	0.5000000000000000	0.1186794254639085
0.8413380683975608	0.5000000000000000	0.0129677334705208
0.1576530278284396	0.5000000000000000	0.0085847196109069
0.6576508326276506	0.0000000000000000	0.0085853448953256
0.8746092740054345	0.5000000000000000	0.6186621576973091
0.3746098812024810	0.0000000000000000	0.6186612433938323
0.6361293986206771	0.5000000000000000	0.5130262559045230
0.8285822159283694	0.0000000000000000	0.5086010504634180

0.1361277686606419	0.0000000000000000	0.5130315100919057
0.3285799161240430	0.5000000000000000	0.5086027940091147
0.0798886007992591	0.5000000000000000	0.4130136222319095
0.5798865970207930	0.0000000000000000	0.4130086516396975
0.8746864962086320	0.0000000000000000	0.3574717560594726
0.3746872380750226	0.5000000000000000	0.3574763855362318
0.8084839877908565	0.5000000000000000	0.2604789274839261
0.6308585522579770	0.0000000000000000	0.2574883696471029
0.1308573659441201	0.5000000000000000	0.2574908537849279
0.0692238211485029	0.0000000000000000	0.1605355722524982
0.5692271264839133	0.5000000000000000	0.1605329400624317
0.8445542676006303	0.0000000000000000	0.8131105035236058
0.8473752065750788	0.0000000000000000	0.6984442922851922
0.1762957215582607	0.0000000000000000	0.9502519459121699
0.5090224395257419	0.0000000000000000	0.9405727827796021
0.3445587194039820	0.5000000000000000	0.8131083131273610
0.3473791908797700	0.5000000000000000	0.6984414763880713
0.6762854535910450	0.5000000000000000	0.9502552121719433
0.0090286803360759	0.5000000000000000	0.9405684706473427
0.6933788323607920	0.5000000000000000	0.6994860203892727
0.6855864973931657	0.5000000000000000	0.8117752734209087
0.3305436789080236	0.5000000000000000	0.956600486073929
0.0240204347013900	0.5000000000000000	0.6929407020939569
0.0078153569674941	0.5000000000000000	0.8215703851547179
0.1933801919974687	0.0000000000000000	0.6994866761605234
0.1855912500719178	0.0000000000000000	0.8117739039558858
0.8305429106050511	0.0000000000000000	0.9565974533511202
0.5240233166807772	0.0000000000000000	0.6929360719784438
0.5078103394831213	0.0000000000000000	0.8215716350842869
0.1693932961816605	0.0000000000000000	0.0617417866541790
0.6693920527898070	0.5000000000000000	0.0617425201098111
0.9912183920410610	0.5000000000000000	0.0793272670896769
0.3365261639774649	0.5000000000000000	0.0647521548546112
0.4912130946483882	0.0000000000000000	0.0793329039261096
0.8365312195429068	-0.0000000000000000	0.0647472967574179
0.8536302905795293	0.0000000000000000	0.5793417799591724
0.2106438853888785	0.0000000000000000	0.5617591306877522
0.3536295128178813	0.5000000000000000	0.5793428350471629
0.7106467702401340	0.5000000000000000	0.5617551316560312
0.5374614828991277	0.0000000000000000	0.5648217230803189
0.0374576550750667	0.5000000000000000	0.5648267178653078
0.9266000313099781	0.5000000000000000	0.4502594925749930
0.7596234553612085	0.0000000000000000	0.4566178360855897
0.6130364420236154	0.5000000000000000	0.4406943359736974
0.2596205444666596	0.5000000000000000	0.4566215728772801
0.4265972175512177	0.0000000000000000	0.4502591499300899
0.1130364617835197	0.0000000000000000	0.4406984808621490
0.6945761301249872	0.0000000000000000	0.3118076410523418
0.8527254800833070	0.5000000000000000	0.3216232201707466
0.5329332560167562	0.5000000000000000	0.3131617673397393
0.3527263240605557	0.0000000000000000	0.3216262384707540
0.1945746858569229	0.5000000000000000	0.3118116593663487
0.0329311739250816	0.0000000000000000	0.3131616263245431
0.7593804149925838	0.5000000000000000	0.1984350911984143
0.4112891717597145	0.5000000000000000	0.1995121932694209
0.2593776497190456	0.0000000000000000	0.1984400864043376
0.9112929568544633	0.0000000000000000	0.1995079316228027
0.5937112691001123	0.0000000000000000	0.1929562504727728
0.0937073922283184	0.5000000000000000	0.1929592463290744

4. (100)-SF 4

(100)SF 4

1.0000000000000000

48.4506950378000028 0.0000000000000000 0.0000000000000000

0.0000000000000000 3.1001288891000001 0.0000000000000000

-0.0021101511000000 -0.0000015765000000 5.9196730666999997

Ga 0

32 48

Direct

0.2265438590000031 0.0003764579999981 0.7522962689999986
0.4596000909999987 0.5003809930000003 0.7369344829999989
0.1642120480000031 0.0003318699999966 0.9910647270000013
0.4765079619999995 0.0003720360000017 0.2530177829999971
0.3972668649999989 0.5003908280000005 0.5004702210000005
0.3515586560000017 0.5003949399999996 0.0045817060000033
0.2892239090000004 0.5003859400000010 0.7679912449999975
0.4141496720000006 0.0003914269999967 0.0145152719999970
0.5222844480000006 0.0003685650000023 0.7519161700000012
0.6471726890000014 0.5002940890000005 0.5007967350000015
0.6015018220000030 0.5003067849999994 0.9987310770000022
0.5391696690000032 0.5003562570000000 0.2357728630000011
0.7096451520000002 0.5002294180000035 0.2629602250000005
0.5846212510000015 0.0003232859999969 0.5127714870000020
0.7722019549999999 0.0001977129999986 0.2510598599999980
0.8346697090000035 0.0001588760000004 0.0132739880000017
0.7265845539999987 0.0002084710000005 0.7490240340000014
0.6640821700000004 0.0002736730000024 0.9867909550000036
0.9766277669999965 0.0001984689999972 0.2499416320000023
0.8972166180000016 0.5001534820000018 0.0015099479999989
0.8516064290000003 0.5001537799999980 0.4992600080000003
0.7891393900000025 0.5001822709999999 0.7370364670000029
0.9596806169999965 0.5001842980000006 0.7639293670000029
0.9141566159999996 0.0001596119999974 0.4874989690000007
0.0222358680000028 0.0002118780000018 0.7529654499999978
0.1473174540000031 0.5003142360000012 0.5050592420000015
0.1016584260000002 0.5003020170000028 0.0017037960000010
0.0391886049999997 0.5002319809999989 0.2390564680000011
0.2096498009999976 0.5003638270000010 0.2684226630000026
0.0847333970000008 0.0002801779999970 0.5156707169999990
0.2723166050000003 0.0003807780000002 0.2518903019999996
0.3346773390000024 0.0003906210000011 0.4905287329999979
0.1660787169999978 0.5003271100000006 0.7829021220000030
0.2484907360000008 0.5003765229999999 0.7542183400000013
0.2925961319999999 0.0003847460000017 0.5295442939999973
0.4562301039999994 0.0003828729999995 0.9753649829999986
0.4177146549999975 0.5003875490000027 0.7775422329999984
0.2914847429999980 0.0003846910000007 0.9758809209999981
0.4573358889999994 0.0003789690000033 0.5290164350000026
0.4160299600000030 0.5003914240000000 0.2227129039999980
0.3327964839999993 0.5003895159999985 0.2823363239999992
0.4984540339999981 0.5003703830000035 0.2505866589999997
0.3734411000000009 0.0003944939999982 0.9953605529999976
0.3753851649999973 0.0003899350000012 0.5097311740000023
0.5414390560000015 0.0003583439999986 0.0280364750000004
0.7078178519999980 0.0002252660000011 0.4712511299999989
0.5827497840000007 0.5003187060000016 0.7208766339999997
0.5425481799999972 0.0003472779999996 0.4742633400000003
0.7060225609999975 0.0002398230000011 0.0252935870000002
0.6677108410000017 0.5002627969999978 0.2244402019999967
0.5810545089999977 0.5003310439999993 0.2757354379999981
0.5003359910000000 0.5003685360000034 0.7503302690000027
0.6233959200000001 0.0003047430000009 0.0072072359999993
0.6252909299999985 0.0002951379999985 0.4921901519999992
0.8328385949999983 0.5001571769999984 0.2215247299999987
0.7503138180000022 0.5001993779999978 0.2424279299999981
0.6659287210000002 0.5002771620000033 0.7785862089999966
0.7484734650000036 0.5002071259999994 0.7576515670000035
0.7909729479999967 0.0001850740000009 0.5287874939999995
0.9578514700000014 0.0001872930000033 0.9722211360000017
0.9159857630000019 0.5001575949999975 0.2792471349999985
0.7927504780000021 0.0001772809999991 0.9747433659999984
0.9560736419999998 0.0001784880000031 0.5262269970000020
0.9177648430000005 0.5001662969999998 0.7252148390000031
0.8310593369999992 0.5001652839999977 0.7755752799999982
0.9985132810000010 0.5002000329999987 0.2589048150000011
0.8734917040000028 0.0001543670000004 0.5079452989999993
0.8753329520000008 0.0001540169999998 0.9927404519999996
0.0410153979999990 0.0002271660000019 0.0307133199999967

0.2073803839999968	0.0003653050000025	0.4761914010000012
0.0828882899999996	0.5002847909999986	0.7239403129999999
0.0428001470000012	0.0002430130000022	0.4767304359999969
0.2062792629999990	0.0003551069999972	0.0299203770000034
0.1677706389999969	0.5003383760000020	0.2280949800000016
0.0811158570000003	0.5002671479999989	0.2780189510000000
0.0003506830000006	0.5002104639999985	0.7438793780000026
0.1235359530000011	0.0003032219999994	0.0108498969999999
0.1254270080000026	0.0003122000000033	0.4960822760000028
0.3311110439999965	0.5003883239999993	0.7274965639999991
0.2503695790000009	0.5003794429999999	0.2541206180000017

5. (001)-SF

(001)SF

1.000000000000000

12.2898233979997968	0.0294924248223792	0.0473335698621348
0.0074126599818637	3.0611543539484902	-0.0640620647798825
-3.5280700754955485	-0.3082474031441104	14.2585590140175604

Ga O

20 30

Direct

0.6714183539054177	0.1070732636683199	0.5227252407587157
0.0967663125084497	0.0455257817776767	0.3170088184327835
0.9129326576327764	0.9968493460352228	0.0802612757641295
0.5967662103150480	0.5455268086691626	0.3170088912218964
0.4129325787617581	0.4968503096915029	0.0802617547223743
0.1647089637908809	0.5040670630249507	0.1249093774868158
0.8451037227144973	0.5314173421896654	0.2718395800943346
0.6647087059321111	0.0040678350129539	0.1249093617861621
0.3451032835355193	0.0314175333278052	0.2718398361289385
0.0979658427367005	0.9625504097200293	0.9185452300384082
0.9162656038098023	0.9210111671204793	0.6855972419808759
0.5979657330074886	0.4625519548988712	0.9185451927074632
0.4162644301268368	0.4210075552776386	0.6855967377472733
0.1659750270575978	0.4267621966330546	0.7255918334520863
0.8451932527633690	0.4552539752332910	0.8745438238005002
0.6659744457985517	0.9267610251367530	0.7255912695588947
0.3451937034417525	0.9552546674841672	0.8745441036120223
0.9189391648428522	0.0474467810015787	0.4769837782816656
0.4189384523427092	0.5474484194286967	0.4769832672739320
0.1714180525902852	0.6070726433126593	0.5227253377793922
0.1761804113439052	0.9874010247051270	0.0439826765959026
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6. (-201)-SF 1

(-201)SF 1

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Ga O

28 42

Direct

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