Electronic supplementary information (ESI)

Selective Kinetic Growth and Role of Local Coordination in Forming Al_2TiO_5-based Coatings at Lower Temperatures

Sebastian Öhman,*[a] Ren Qiu,[b] Tomas Edvinsson,[c] Olof Bäcke [b], Tobias Törndahl,[c] Mats Boman[a]

Supplementary figures

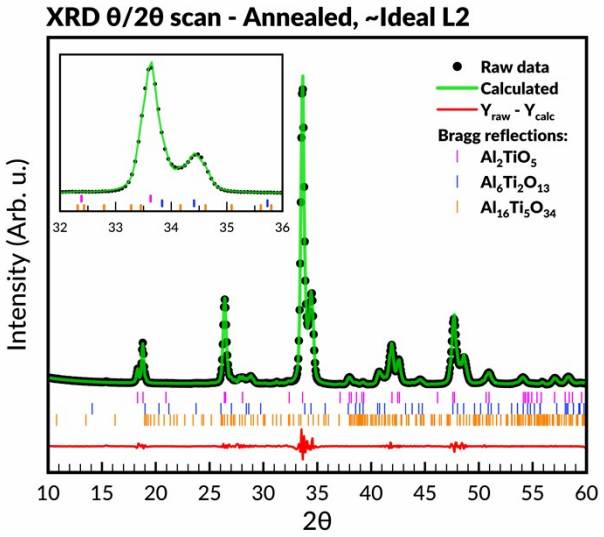

Figure S1 –Pawley refined diffractogram of annealed batch L2, corresponding to a near-to-ideal Al:Ti composition (1.88) for Al_2TiO_5. Calculated green line from the presence of Al_2TiO_5 and the two intergrowths $Al_6Ti_2O_{13}$; $Al_{16}Ti_5O_{34}$. Bragg reflections marked for all three phases.

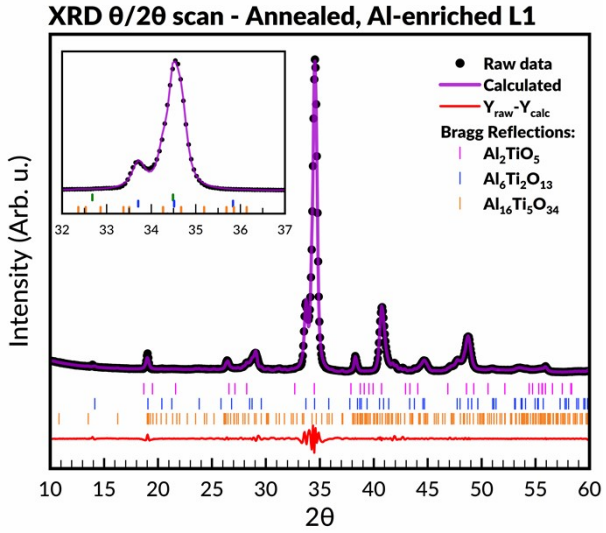

Figure S2 Pawley refined diffractogram of Annealed batch L1, corresponding to an Al-enriched Al:Ti composition (3.29). Calculated purple line from the presence of Al_2TiO_5 and the two intergrowths $Al_6Ti_2O_{13}$; $Al_{16}Ti_5O_{34}$. Bragg reflections marked for all three phases.

Structural reports and corresponding hkl values – L2 ideal composition

[a] *Inorganic Chemistry, Department of Chemistry – Ångström Laboratory, Uppsala University, Box 538, Uppsala SE-75121, Sweden*
[b] *Department of Physics, Chalmers University of Technology, Gothenburg SE-41296, Sweden*
[c] *Department of Materials Science and Engineering, Ångström Laboratory, Uppsala University, Box 35, Uppsala SE-75103, Sweden*
*Corresponding Author

hkl Phase - 1 Pawley method

Phase name	Al_2TiO_5
R-Bragg	0.171
Spacegroup	Cmcm
Cell Volume (Å^3)	328.65(18)
Lattice parameters	
a (Å)	3.6003(18)
b (Å)	9.4292(17)
c (Å)	9.6809(11)

h	k	l	m	d	Th2	I
0	0	2	2	4.84046	18.31366	69(3)
0	2	0	2	4.71458	18.80702	217(9)
0	2	1	4	4.23866	20.94124	1(3)
0	2	2	4	3.37734	26.36794	680(170)
1	1	0	4	3.36348	26.47858	430(50)
1	1	1	8	3.17718	28.06204	60(30)
1	1	2	8	2.76211	32.38677	0(80)
0	2	3	4	2.66293	33.62822	5300(180)
0	0	4	2	2.42023	37.11724	11(19)
1	3	0	4	2.36774	37.97115	0(4000)
0	4	0	2	2.35729	38.14602	0(5000)
1	1	3	8	2.32858	38.63494	8(20000)
1	3	1	8	2.29995	39.13525	8(2000)
0	4	1	4	2.29037	39.30573	0(1700)
0	2	4	4	2.15310	41.92568	1230(130)
1	3	2	8	2.12692	42.46658	530(70)
0	4	2	4	2.11933	42.62601	550(60)
1	1	4	8	1.96451	46.17139	10(20)
1	3	3	8	1.90899	47.59557	3(700)
0	4	3	4	1.90350	47.74139	1580(180)

2	0	0	2	1.80016	50.66937	300(400)
0	2	5	4	1.79103	50.94612	8(1200)
1	3	4	8	1.69250	54.14592	0(13000)
0	4	4	4	1.68867	54.27881	0(18000)
2	0	2	4	1.68726	54.32794	0(3000)
2	2	0	4	1.68174	54.52102	0(1700)
1	1	5	8	1.67802	54.65192	0(30000)
1	5	0	4	1.67054	54.91719	0(400)
2	2	1	8	1.65692	55.40709	0(14000)
1	5	1	8	1.64621	55.79902	0(6000)
0	0	6	2	1.61349	57.03304	310(150)
2	2	2	8	1.58859	58.01110	0(1000)
1	5	2	8	1.57914	58.39162	0(2000)
0	6	0	2	1.57153	58.70208	0(8000)
0	6	1	4	1.55122	59.54737	0(4000)

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hkl Phase - 2 Pawley method

Phase name	$Al_6Ti_2O_{13}$
R-Bragg	0.305
Spacegroup	Cm2m
Cell Volume (Å^3)	430.3(2)
Lattice parameters	
a (Å)	3.6727(14)
b (Å)	9.331(3)
c (Å)	12.555(3)

h	k	l	m	d	Th2	I
0	0	2	2	6.27734	14.09716	0.0(14)
0	2	0	2	4.66562	19.00620	0(70)
0	2	1	4	4.37339	20.28919	0(10)
0	0	3	2	4.18490	21.21339	0(4)
0	2	2	4	3.74460	23.74203	4(4)
1	1	0	4	3.41753	26.05232	0(40)
1	1	1	8	3.29754	27.01793	60(90)
0	0	4	2	3.13867	28.41351	19(13)
0	2	3	4	3.11531	28.63115	94(13)
1	1	2	8	3.00154	29.74092	7(7)
1	1	3	8	2.64703	33.83622	2010(150)
0	2	4	4	2.60423	34.40950	2290(140)
0	0	5	2	2.51094	35.73022	0(50)
1	3	0	4	2.37358	37.87425	200(400)
0	4	0	2	2.33281	38.56206	0(110000)
1	3	1	8	2.33226	38.57146	0(110000)
1	1	4	8	2.31168	38.92858	0(20000)
0	4	1	4	2.29355	39.24893	0(5000)
1	3	2	8	2.22017	40.60239	240(110)
0	2	5	4	2.21107	40.77685	400(300)
0	4	2	4	2.18670	41.25193	200(400)

0	0	6	2	2.09245	43.20098	90(40)
1	3	3	8	2.06461	43.81332	110(20)
0	4	3	4	2.03761	44.42456	200(50)
1	1	5	8	2.02349	44.75133	90(190)
0	2	6	4	1.90923	47.58930	3100(1000)
1	3	4	8	1.89318	48.01805	1(500)
0	4	4	4	1.87230	48.58793	1800(300)
2	0	0	2	1.83636	49.60224	0(400)
2	0	1	4	1.81703	50.16632	0(120)
0	0	7	2	1.79353	50.87013	500(500)
1	1	6	8	1.78453	51.14510	150(130)
2	0	2	4	1.76249	51.83165	0(60)
1	3	5	8	1.72489	53.04872	0(300)
0	4	5	4	1.70905	53.57934	0(50000)
2	2	0	4	1.70877	53.58899	0(60000)
2	2	1	8	1.69316	54.12318	0(12000)
2	0	3	4	1.68159	54.52629	0(3000)
0	2	7	4	1.67409	54.79079	0(2000)
1	5	0	4	1.66377	55.15952	0(700)
1	5	1	8	1.64935	55.68346	0(110000)
2	2	2	8	1.64877	55.70475	1(120000)
1	5	2	8	1.60824	57.23616	300(700)
1	1	7	8	1.58811	58.03010	0(2000)
2	0	4	4	1.58501	58.15477	200(1700)
2	2	3	8	1.58197	58.27703	600(1800)
1	3	6	8	1.56962	58.78057	0(9000)
0	0	8	2	1.56934	58.79205	0(7000)
0	4	6	4	1.55765	59.27684	200(1000)
0	6	0	2	1.55521	59.37944	100(1200)
1	5	3	8	1.54607	59.76600	0(400000)

hkl Phase - 3 Pawley method

Phase name	$Al_{16}Ti_5O_{34}$
R-Bragg	0.193
Spacegroup	Cmcm
Cell Volume (Å^3)	2234.0(7)
Lattice parameters	
a (Å)	3.6723(8)
b (Å)	9.2883(18)
c (Å)	65.494(10)

h	k	l	m	d	Th2	I
0	0	8	2	8.18676	10.79798	0.0(8)
0	0	10	2	6.54941	13.50877	0.0(10)
0	0	12	2	5.45784	16.22718	0.5(13)
0	0	14	2	4.67815	18.95483	2(40)
0	2	0	2	4.64413	19.09494	9(30)
0	2	1	4	4.63250	19.14334	0(9)
0	2	2	4	4.59812	19.28782	0(5)
0	2	3	4	4.54249	19.52635	0(2)
0	2	4	4	4.46789	19.85566	0(2)
0	2	5	4	4.37716	20.27151	0(8)
0	2	6	4	4.27344	20.76893	0(2)
0	2	7	4	4.15987	21.34250	0(3)
0	0	16	2	4.09338	21.69335	0(2)
0	2	8	4	4.03945	21.98656	0(2)
0	2	9	4	3.91485	22.69549	0(3)
0	2	10	4	3.78837	23.46378	0(3)
0	2	11	4	3.66191	24.28623	1(3)
0	0	18	2	3.63856	24.44448	0(3)

0	2	12	4	3.53696	25.15799	4(3)
1	1	0	4	3.41508	26.07140	0(10000)
0	2	13	4	3.41466	26.07460	0(10000)
1	1	1	8	3.41044	26.10744	0(1100)
1	1	2	8	3.39665	26.21530	130(70)
1	1	3	8	3.37404	26.39415	0(180)
1	1	4	8	3.34313	26.64267	123(18)
1	1	5	8	3.30461	26.95907	0(40)
0	2	14	4	3.29586	27.03201	6(30)
0	0	20	2	3.27470	27.20999	0(13)
1	1	6	8	3.25929	27.34118	31(6)
1	1	7	8	3.20806	27.78650	69(6)
0	2	15	4	3.18112	28.02658	20(30)
1	1	8	8	3.15184	28.29231	38(9)
1	1	9	8	3.09157	28.85572	73(8)
0	2	16	4	3.07081	29.05508	42(6)
1	1	10	8	3.02813	29.47375	6(5)
0	0	22	2	2.97700	29.99175	2(9)
0	2	17	4	2.96514	30.11460	0(30)
1	1	11	8	2.96237	30.14339	9(30)
1	1	12	8	2.89504	30.86167	8(5)
0	2	18	4	2.86418	31.20263	31(6)
1	1	13	8	2.82682	31.62570	10(6)
0	2	19	4	2.76792	32.31690	20(30)
1	1	14	8	2.75830	32.43269	0(50)
0	0	24	2	2.72892	32.79173	0(7)
1	1	15	8	2.68999	33.28000	0(40)
0	2	20	4	2.67628	33.45547	1620(130)
1	1	16	8	2.62230	34.16513	480(70)
0	2	21	4	2.58912	34.61663	590(70)
1	1	17	8	2.55557	35.08574	0(10)

0	0	26	2	2.51900	35.61198	0(20)
0	2	22	4	2.50628	35.79889	3(30)
1	1	18	8	2.49008	36.03968	1(8)
0	2	23	4	2.42757	37.00095	7(50)
1	1	19	8	2.42605	37.02494	0(60)
1	3	0	4	2.36708	37.98214	0(10000)
1	3	1	8	2.36554	38.00788	0(13000)
1	1	20	8	2.36363	38.03972	9(2000)
1	3	2	8	2.36092	38.08504	0(6000)
1	3	3	8	2.35329	38.21335	3(13000)
0	2	24	4	2.35280	38.22170	0(16000)
1	3	4	8	2.34273	38.39237	20(60)
0	0	28	2	2.33907	38.45472	0(1100)
1	3	5	8	2.32936	38.62151	0(17000)
0	4	0	2	2.32207	38.74755	0(18000)
0	4	1	4	2.32061	38.77287	6(20000)
0	4	2	4	2.31625	38.84875	0(5000)
1	3	6	8	2.31332	38.90002	0(5000)
0	4	3	4	2.30904	38.97493	0(9000)
1	1	21	8	2.30294	39.08234	0(1100)
0	4	4	4	2.29906	39.15100	0(2000)
1	3	7	8	2.29478	39.22701	1(90)
0	4	5	4	2.28642	39.37642	1(1000)
0	2	25	4	2.28176	39.46019	5(130)
1	3	8	8	2.27394	39.60150	10(50)
0	4	6	4	2.27125	39.65046	0(40)
0	4	7	4	2.25370	39.97231	10(50)
1	3	9	8	2.25099	40.02238	0(40)
1	1	22	8	2.24406	40.15129	1(17)
0	4	8	4	2.23395	40.34102	1(20)
1	3	10	8	2.22615	40.48845	10(40)

0	2	26	4	2.21425	40.71560	0(300)
0	4	9	4	2.21218	40.75554	10(140)
1	3	11	8	2.19963	40.99848	140(60)
0	4	10	4	2.18858	41.21474	0(190)
1	1	23	8	2.18704	41.24522	60(130)
0	0	30	2	2.18314	41.32227	0(130)
1	3	12	8	2.17164	41.55115	600(50)
0	4	11	4	2.16336	41.71745	160(40)
0	2	27	4	2.15009	41.98723	0(120)
1	3	13	8	2.14239	42.14514	20(60)
0	4	12	4	2.13672	42.26241	210(50)
1	1	24	8	2.13188	42.36289	120(90)
1	3	14	8	2.11210	42.77910	110(50)
0	4	13	4	2.10885	42.84837	10(60)
0	2	28	4	2.08906	43.27452	0(40)
1	3	15	8	2.08095	43.45169	0(1700)
0	4	14	4	2.07994	43.47404	0(1000)
1	1	25	8	2.07861	43.50322	0(700)
0	4	15	4	2.05017	44.13812	50(110)
1	3	16	8	2.04914	44.16156	0(140)
0	0	32	2	2.04669	44.21715	10(60)
0	2	29	4	2.03100	44.57697	60(50)
1	1	26	8	2.02719	44.66524	0(90)
0	4	16	4	2.01972	44.83934	30(100)
1	3	17	8	2.01682	44.90742	30(40)
0	4	17	4	1.98876	45.57645	20(20)
1	3	18	8	1.98416	45.68798	0(30)
1	1	27	8	1.97761	45.84809	5(50)
0	2	30	4	1.97573	45.89421	7(60)
0	4	18	4	1.95742	46.34821	0(19)
1	3	19	8	1.95131	46.50202	0(19)

1	1	28	8	1.92981	47.05101	0(1000)
0	0	34	2	1.92630	47.14206	0(40)
0	4	19	4	1.92586	47.15342	0(900)
0	2	31	4	1.92307	47.22593	0(200)
1	3	20	8	1.91838	47.34834	320(120)
0	4	20	4	1.89419	47.99096	700(400)
1	3	21	8	1.88551	48.22583	0(190)
1	1	29	8	1.88376	48.27336	550(160)
0	2	32	4	1.87288	48.57190	0(300)
0	4	21	4	1.86252	48.85971	310(50)
1	3	22	8	1.85278	49.13340	30(30)
1	1	30	8	1.83941	49.51458	0(100)
2	0	0	2	1.83615	49.60823	10(70)
2	0	2	4	1.83327	49.69143	0(600)
0	4	22	4	1.83095	49.75866	7(160)
0	2	33	4	1.82500	49.93196	4(90)
2	0	4	4	1.82472	49.94041	30(160)
1	3	23	8	1.82029	50.07006	0(170)
0	0	36	2	1.81928	50.09991	0(600)
2	0	6	4	1.81071	50.35338	0(300)
0	4	23	4	1.79958	50.68681	120(40)
1	1	31	8	1.79669	50.77418	0(170)
2	0	8	4	1.79164	50.92742	200(300)
1	3	24	8	1.78812	51.03485	0(1100)
0	2	34	4	1.77931	51.30601	50(50)
0	4	24	4	1.76848	51.64325	0(200)
2	0	10	4	1.76799	51.65870	0(300)
1	3	25	8	1.75634	52.02692	2(130)
1	1	32	8	1.75556	52.05179	0(130)
2	0	12	4	1.74031	52.54258	0(90)
0	4	25	4	1.73771	52.62712	0(70)

0	2	35	4	1.73566	52.69402	0(60)
1	3	26	8	1.72499	53.04543	0(190)
0	0	38	2	1.72353	53.09390	7(80)
1	1	33	8	1.71594	53.34708	30(180)
2	0	14	4	1.70921	53.57390	0(5000)
2	2	0	4	1.70754	53.63065	0(800)
0	4	26	4	1.70733	53.63763	0(4000)
2	2	1	8	1.70696	53.65033	9(1700)
2	2	2	8	1.70522	53.70935	0(1000)
2	2	3	8	1.70234	53.80762	0(60000)
2	2	4	8	1.69833	53.94499	0(50000)
1	3	27	8	1.69413	54.08965	0(500)
0	2	36	4	1.69394	54.09602	200(400)
2	2	5	8	1.69321	54.12125	0(4000)
2	2	6	8	1.68702	54.33616	0(9000)
2	2	7	8	1.67979	54.58940	0(13000)
1	1	34	8	1.67780	54.65980	7(30000)
0	4	27	4	1.67739	54.67404	0(3000)
2	0	16	4	1.67532	54.74714	0(1300)
2	2	8	8	1.67157	54.88061	0(200)
1	3	28	8	1.66379	55.15889	0(300)
2	2	9	8	1.66239	55.20939	0(6000)
1	5	0	4	1.65764	55.38120	0(3000)
1	5	1	8	1.65711	55.40045	0(50000)
1	5	2	8	1.65552	55.45821	0(1300000)
0	2	37	4	1.65404	55.51207	6(500000)
1	5	3	8	1.65288	55.55437	0(200)
2	2	10	8	1.65230	55.57531	0(15000)
1	5	4	8	1.64921	55.68881	0(12000)
0	4	28	4	1.64793	55.73571	0(4000)
1	5	5	8	1.64452	55.86135	0(900000)

2	2	11	8	1.64137	55.97790	0(3000)
1	1	35	8	1.64105	55.98979	0(8000)
2	0	18	4	1.63925	56.05663	0(1100)
1	5	6	8	1.63885	56.07176	0(300)
0	0	40	2	1.63735	56.12749	0(700)
1	3	29	8	1.63401	56.25256	0(10000)
1	5	7	8	1.63222	56.31975	0(3000)
2	2	12	8	1.62964	56.41665	0(300)
1	5	8	8	1.62467	56.60501	130(140)
0	4	29	4	1.61898	56.82202	0(200)
2	2	13	8	1.61718	56.89104	0(90000)
1	5	9	8	1.61624	56.92718	0(70000)
0	2	38	4	1.61584	56.94231	0(1500)
1	5	10	8	1.60697	57.28585	5(30000)
1	1	36	8	1.60566	57.33693	0(3000)
1	3	30	8	1.60481	57.37011	0(3000)
2	2	14	8	1.60403	57.40051	60(180)
2	0	20	4	1.60157	57.49677	0(900)
1	5	11	8	1.59690	57.68062	0(1800)
0	4	30	4	1.59056	57.93245	40(140)
2	2	15	8	1.59026	57.94452	0(600)
1	5	12	8	1.58610	58.11102	0(1700)
0	2	39	4	1.57926	58.38691	100(1800)
1	3	31	8	1.57620	58.51105	0(1200)
2	2	16	8	1.57592	58.52250	0(3000)
1	5	13	8	1.57459	58.57657	0(6000)
1	1	37	8	1.57155	58.70116	0(3000)
2	0	22	4	1.56280	59.06216	0(14000000)
0	4	31	4	1.56270	59.06652	0(4000000)
1	5	14	8	1.56245	59.07679	0(200)
2	2	17	8	1.56108	59.13387	0(500000)

0	0	42	2	1.55938	59.20454	0(10000000)
1	5	15	8	1.54971	59.61116	0(300000)
1	3	32	8	1.54821	59.67498	0(300)
0	6	0	2	1.54804	59.68191	0(300000)
0	6	1	4	1.54761	59.70027	0(14000)
0	6	2	4	1.54632	59.75533	0(100000)
2	2	18	8	1.54578	59.77805	0(400000)
0	2	40	4	1.54419	59.84609	0(600000)
0	6	3	4	1.54417	59.84703	0(80000)
0	6	4	4	1.54117	59.97527	0(3000000)
1	1	38	8	1.53868	60.08250	0(4000000)
0	6	5	4	1.53735	60.13991	0(7000000)
1	5	16	8	1.53644	60.17917	0(100000)
0	4	32	4	1.53540	60.22382	0(6000000)
0	6	6	4	1.53271	60.34076	0(600000)

Structural reports and corresponding hkl values – L1 Al-enriched

hkl Phase - 1 Pawley method

Phase name	Al_2TiO_5
R-Bragg	1.117
Spacegroup	Cmcm
Lattice parameters	
a (Å)	3.605(6)
b (Å)	9.106(14)
c (Å)	9.493(7)

h	k	l	m	d	Th2	I
0	0	2	2	4.74656	18.67916	0(5)
0	2	0	2	4.55290	19.48127	0(11)
0	2	1	4	4.10519	21.63021	2(6)
1	1	0	4	3.35192	26.57156	0(20)
0	2	2	4	3.28572	27.11703	9(110)
1	1	1	8	3.16068	28.21156	60(20)
1	1	2	8	2.73803	32.67959	9(15)
0	2	3	4	2.59842	34.48890	4000(5000)
0	0	4	2	2.37328	37.87918	0(50)
1	3	0	4	2.32189	38.75064	0(16000)
1	1	3	8	2.30100	39.11678	1(1200)
0	4	0	2	2.27645	39.55602	0(800)
1	3	1	8	2.25541	39.94070	0(190)
0	4	1	4	2.21369	40.72638	1000(4000)
0	2	4	4	2.10452	42.94081	0(200)
1	3	2	8	2.08572	43.34747	0(1500)
0	4	2	4	2.05259	44.08330	70(130)
1	1	4	8	1.93693	46.86783	90(50)
1	3	3	8	1.87200	48.59610	600(500)
0	4	3	4	1.84794	49.27058	0(400)

2	0	0	2	1.80253	50.59819	0(200)
0	2	5	4	1.75236	52.15385	0(800)
2	0	2	4	1.68511	54.40290	0(400)
2	2	0	4	1.67596	54.72472	0(4000)
1	3	4	8	1.65970	55.30660	0(14000)
1	1	5	8	1.65201	55.58597	0(300000)
2	2	1	8	1.65044	55.64372	0(500000)
0	4	4	4	1.64286	55.92279	0(80000)
1	5	0	4	1.62552	56.57261	0(1000)
1	5	1	8	1.60220	57.47201	0(7000)
0	0	6	2	1.58219	58.26836	0(400)
2	2	2	8	1.58034	58.34304	3(500)
1	5	2	8	1.53784	60.11857	0(2000000)
0	6	0	2	1.51763	61.00356	0(1600000)
0	6	1	4	1.49860	61.86264	300000(1900000)

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hkl Phase - 2 Pawley method

Phase name	Al6Ti2O13
R-Bragg	1.538
Spacegroup	Cm2m
Cell Volume (Å^3)	432.0(12)
Lattice parameters	
a (Å)	3.709(3)
b (Å)	9.30(2)
c (Å)	12.519(16)

h	k	l	m	d	Th2	I
0	0	2	2	6.25967	14.13716	4.2(18)
0	2	0	2	4.65101	19.06644	0(200)
0	2	1	4	4.35987	20.35279	3(9)
0	0	3	2	4.17311	21.27398	4(9)
0	2	2	4	3.73329	23.81496	11(5)
1	1	0	4	3.44540	25.83794	5(7)
1	1	1	8	3.32190	26.81614	20(30)
0	0	4	2	3.12984	28.49542	40(40)
0	2	3	4	3.10610	28.71785	140(20)
1	1	2	8	3.01839	29.57108	40(90)
1	1	3	8	2.65688	33.70699	1530(110)
0	2	4	4	2.59664	34.51320	0(6000)
0	0	5	2	2.50387	35.83451	0(400)
1	3	0	4	2.37895	37.78540	30(50)
1	3	1	8	2.33713	38.48790	3(10000)
0	4	0	2	2.32551	38.68797	0(5000)
1	1	4	8	2.31668	38.84134	0(30000)
0	4	1	4	2.28640	39.37683	0(8000)
1	3	2	8	2.22377	40.53360	0(1100)
0	2	5	4	2.20469	40.90015	1200(600)
0	4	2	4	2.17993	41.38575	0(3000)

0	0	6	2	2.08656	43.32910	0(500)
1	3	3	8	2.06672	43.76629	140(70)
0	4	3	4	2.03139	44.56802	300(300)
1	1	5	8	2.02549	44.70470	200(1600)
0	2	6	4	1.90376	47.73468	510(130)
1	3	4	8	1.89395	47.99723	0(600)
0	4	4	4	1.86665	48.74458	1300(1000)
2	0	0	2	1.85461	49.08179	100(300)
2	0	1	4	1.83459	49.65343	0(1000)
0	0	7	2	1.78848	51.02404	0(900)
1	1	6	8	1.78478	51.13742	0(3000)
2	0	2	4	1.77820	51.34021	0(700)
1	3	5	8	1.72464	53.05683	0(1300)
2	2	0	4	1.72270	53.12141	8(3000)
2	2	1	8	1.70662	53.66183	0(4000)
0	4	5	4	1.70395	53.75260	0(30000)
2	0	3	4	1.69478	54.06712	3(3000)
0	2	7	4	1.66931	54.96095	0(14000)
1	5	0	4	1.66296	55.18888	0(30000)
2	2	2	8	1.66095	55.26126	0(110000)
1	5	1	8	1.64848	55.71558	0(200000)
1	5	2	8	1.60721	57.27641	0(800)
2	0	4	4	1.59553	57.73498	0(7000)
2	2	3	8	1.59236	57.86084	0(1400)
1	1	7	8	1.58736	58.06042	0(2000)
1	3	6	8	1.56867	58.81952	0(3000)
0	0	8	2	1.56492	58.97440	300(1800)
0	4	6	4	1.55305	59.47023	0(9000)
0	6	0	2	1.55034	59.58471	0(30000)
1	5	3	8	1.54482	59.81929	0(1400000)
0	6	1	4	1.53859	60.08648	0(3000000)

hkl Phase - 3 Pawley method

Phase name	$Al_{16}Ti_5O_{34}$
R-Bragg	1.389
Spacegroup	Cmcm
Cell Volume (Å^3)	2220(3)
Lattice parameters	
a (Å)	3.658(2)
b (Å)	9.287(10)
c (Å)	65.36(4)

h	k	l	m	d	Th2	I
0	0	8	2	8.16941	10.82097	0.0(12)
0	0	10	2	6.53553	13.53759	1.1(14)
0	0	12	2	5.44627	16.26188	1.9(19)
0	0	14	2	4.66823	18.99545	50(70)
0	2	0	2	4.64347	19.09769	30(120)
0	2	1	4	4.63180	19.14628	0(30)
0	2	2	4	4.59729	19.29136	0(12)
0	2	3	4	4.54145	19.53086	0(11)
0	2	4	4	4.46659	19.86148	0(3)
0	2	5	4	4.37557	20.27896	0(8)
0	2	6	4	4.27153	20.77831	1(3)
0	2	7	4	4.15765	21.35404	0(8)
0	0	16	2	4.08471	21.73997	1(6)
0	2	8	4	4.03692	22.00048	1(4)
0	2	9	4	3.91205	22.71196	2(4)
0	2	10	4	3.78532	23.48295	7(4)
0	2	11	4	3.65864	24.30823	6(5)
0	0	18	2	3.63085	24.49719	4(5)

0	2	12	4	3.53351	25.18292	8(5)
0	2	13	4	3.41107	26.10254	0(60)
1	1	0	4	3.40378	26.15941	0(170)
1	1	1	8	3.39918	26.19550	0(150)
1	1	2	8	3.38547	26.30347	40(40)
1	1	3	8	3.36298	26.48253	80(30)
1	1	4	8	3.33224	26.73133	5(30)
1	1	5	8	3.29393	27.04811	2(400)
0	2	14	4	3.29215	27.06303	0(500)
0	0	20	2	3.26776	27.26888	4(14)
1	1	6	8	3.24886	27.43068	21(10)
1	1	7	8	3.19790	27.87656	29(9)
0	2	15	4	3.17732	28.06075	13(19)
1	1	8	8	3.14197	28.38302	20(30)
1	1	9	8	3.08201	28.94718	100(20)
0	2	16	4	3.06695	29.09243	200(20)
1	1	10	8	3.01889	29.56605	0(70)
0	0	22	2	2.97069	30.05693	10(20)
0	2	17	4	2.96124	30.15519	0(30)
1	1	11	8	2.95345	30.23664	30(20)
1	1	12	8	2.88644	30.95598	26(9)
0	2	18	4	2.86026	31.24648	38(9)
1	1	13	8	2.81853	31.72117	26(9)
0	2	19	4	2.76400	32.36406	22(13)
1	1	14	8	2.75032	32.52943	0(17)
0	0	24	2	2.72314	32.86333	0(13)
1	1	15	8	2.68231	33.37811	0(30)
0	2	20	4	2.67236	33.50597	0(60)
1	1	16	8	2.61490	34.26471	1600(300)
0	2	21	4	2.58522	34.67049	3700(900)
1	1	17	8	2.54845	35.18689	0(30)

0	0	26	2	2.51366	35.69014	0(70)
0	2	22	4	2.50241	35.85614	0(300)
1	1	18	8	2.48323	36.14251	20(20)
0	2	23	4	2.42373	37.06163	40(30)
1	1	19	8	2.41946	37.12955	5(30)
1	3	0	4	2.36314	38.04796	0(800)
1	3	1	8	2.36160	38.07378	0(1300)
1	1	20	8	2.35728	38.14621	0(9000)
1	3	2	8	2.35698	38.15116	0(9000)
1	3	3	8	2.34936	38.27982	0(6000)
0	2	24	4	2.34900	38.28585	0(6000)
1	3	4	8	2.33880	38.45934	0(5000)
0	0	28	2	2.33412	38.53959	0(3000)
1	3	5	8	2.32544	38.68911	0(5000)
0	4	0	2	2.32174	38.75330	0(30000)
0	4	1	4	2.32027	38.77872	0(6000)
0	4	2	4	2.31590	38.85491	6(15000)
1	3	6	8	2.30942	38.96839	0(4000)
0	4	3	4	2.30866	38.98161	0(2000)
0	4	4	4	2.29864	39.15841	0(2000)
1	1	21	8	2.29682	39.19080	0(1700)
1	3	7	8	2.29090	39.29629	0(1400)
0	4	5	4	2.28595	39.38474	0(5000)
0	2	25	4	2.27801	39.52783	9(1500)
0	4	6	4	2.27073	39.65990	0(1100)
1	3	8	8	2.27007	39.67181	0(1000)
0	4	7	4	2.25312	39.98306	0(200)
1	3	9	8	2.24714	40.09385	0(120)
1	1	22	8	2.23816	40.26183	0(110)
0	4	8	4	2.23330	40.35324	0(200)
1	3	10	8	2.22232	40.56121	800(900)

0	4	9	4	2.21146	40.76941	0(14000)
0	2	26	4	2.21055	40.78676	0(10000)
1	3	11	8	2.19583	41.07265	180(180)
0	4	10	4	2.18779	41.23043	100(300)
1	1	23	8	2.18134	41.35793	0(900)
0	0	30	2	2.17851	41.41404	0(1400)
1	3	12	8	2.16786	41.62684	0(200)
0	4	11	4	2.16249	41.73510	230(90)
0	2	27	4	2.14644	42.06196	190(50)
1	3	13	8	2.13865	42.22247	0(110)
0	4	12	4	2.13577	42.28219	0(100)
1	1	24	8	2.12638	42.47787	120(40)
1	3	14	8	2.10839	42.85818	100(1300)
0	4	13	4	2.10781	42.87041	5(1500)
0	2	28	4	2.08547	43.35285	0(2000)
0	4	14	4	2.07882	43.49846	0(800)
1	3	15	8	2.07727	43.53262	0(700)
1	1	25	8	2.07329	43.62056	0(190)
0	4	15	4	2.04898	44.16505	0(300)
1	3	16	8	2.04549	44.24445	0(400)
0	0	32	2	2.04235	44.31601	200(200)
0	2	29	4	2.02746	44.65894	0(1000)
1	1	26	8	2.02205	44.78503	0(700)
0	4	16	4	2.01846	44.86891	0(200)
1	3	17	8	2.01321	44.99237	120(100)
0	4	17	4	1.98742	45.60875	30(40)
1	3	18	8	1.98059	45.77509	7(50)
1	1	27	8	1.97263	45.97042	0(500)
0	2	30	4	1.97224	45.97987	0(500)
0	4	18	4	1.95602	46.38334	30(30)
1	3	19	8	1.94777	46.59137	20(40)

1	1	28	8	1.92499	47.17599	0(4000)
0	4	19	4	1.92439	47.19150	0(5000)
0	0	34	2	1.92221	47.24823	0(2000)
0	2	31	4	1.91965	47.31532	0(900)
1	3	20	8	1.91489	47.44004	120(190)
0	4	20	4	1.89266	48.03206	200(400)
1	3	21	8	1.88205	48.31997	220(160)
1	1	29	8	1.87909	48.40108	200(200)
0	2	32	4	1.86951	48.66507	0(1100)
0	4	21	4	1.86094	48.90394	500(400)
1	3	22	8	1.84937	49.23007	0(500)
1	1	30	8	1.83487	49.64513	0(700)
0	4	22	4	1.82932	49.80609	4(7000)
2	0	0	2	1.82918	49.81021	0(7000)
2	0	2	4	1.82632	49.89352	8(400)
0	2	33	4	1.82169	50.02896	0(200)
2	0	4	4	1.81782	50.14281	4(1300)
1	3	23	8	1.81692	50.16934	4(1700)
0	0	36	2	1.81542	50.21366	4(600)
2	0	6	4	1.80392	50.55632	1(300)
0	4	23	4	1.79790	50.73752	10(120)
1	1	31	8	1.79229	50.90767	0(200)
2	0	8	4	1.78498	51.13113	0(5000)
1	3	24	8	1.78480	51.13684	2(6000)
0	2	34	4	1.77605	51.40690	0(300)
0	4	24	4	1.76676	51.69732	0(160)
2	0	10	4	1.76149	51.86343	0(300)
1	3	25	8	1.75305	52.13169	0(700)
1	1	32	8	1.75128	52.18830	0(400)
0	4	25	4	1.73595	52.68462	0(500)
2	0	12	4	1.73399	52.74861	0(900)

0	2	35	4	1.73246	52.79887	0(500)
1	3	26	8	1.72175	53.15309	0(1500)
0	0	38	2	1.71988	53.21549	0(400)
1	1	33	8	1.71179	53.48671	100(600)
0	4	26	4	1.70554	53.69864	5(5000)
2	0	14	4	1.70310	53.78152	0(20000)
2	2	0	4	1.70189	53.82286	0(30000)
2	2	1	8	1.70132	53.84258	0(20000)
2	2	2	8	1.69959	53.90171	0(2000)
2	2	3	8	1.69672	54.00015	0(2000)
2	2	4	8	1.69273	54.13777	0(3000)
1	3	27	8	1.69093	54.20028	0(20000)
0	2	36	4	1.69080	54.20488	0(20000)
2	2	5	8	1.68765	54.31435	9(600)
2	2	6	8	1.68149	54.52965	0(400)
0	4	27	4	1.67557	54.73864	0(8000)
2	2	7	8	1.67430	54.78335	0(7000)
1	1	34	8	1.67376	54.80267	8(6000)
2	0	16	4	1.66943	54.95666	0(8000)
2	2	8	8	1.66612	55.07510	1(2000)
1	3	28	8	1.66064	55.27258	0(70000)
2	2	9	8	1.65699	55.40450	0(90000)
1	5	0	4	1.65616	55.43481	0(200000)
1	5	1	8	1.65563	55.45414	0(190000)
1	5	2	8	1.65404	55.51210	1(50000)
1	5	3	8	1.65139	55.60861	0(1600000)
0	2	37	4	1.65095	55.62501	0(1900000)
1	5	4	8	1.64772	55.74353	0(70000)
2	2	10	8	1.64697	55.77112	2(90000)
0	4	28	4	1.64608	55.80396	0(60000)
1	5	5	8	1.64302	55.91669	0(120000)

1	5	6	8	1.63734	56.12786	0(60000)
1	1	35	8	1.63712	56.13599	0(80000)
2	2	11	8	1.63609	56.17448	0(20000)
0	0	40	2	1.63388	56.25726	4(20000)
2	0	18	4	1.63358	56.26840	0(19000)
1	3	29	8	1.63090	56.36940	0(12000)
1	5	7	8	1.63070	56.37674	0(10000)
2	2	12	8	1.62443	56.61409	7(1400)
1	5	8	8	1.62314	56.66302	0(1000)
0	4	29	4	1.61710	56.89400	0(500)
1	5	9	8	1.61470	56.98634	5(500)
0	2	38	4	1.61280	57.05941	0(1200)
2	2	13	8	1.61203	57.08941	7(1100)
1	5	10	8	1.60541	57.34630	0(1000)
1	1	36	8	1.60183	57.48656	3(50000)
1	3	30	8	1.60174	57.49018	2(50000)
2	2	14	8	1.59895	57.59991	1(1300)
2	0	20	4	1.59613	57.71116	0(1600)
1	5	11	8	1.59534	57.74247	0(4000)
0	4	30	4	1.58866	58.00823	1(1000)
2	2	15	8	1.58525	58.14503	0(2000)
1	5	12	8	1.58452	58.17441	0(1600)
0	2	39	4	1.57627	58.50824	0(600)
1	3	31	8	1.57318	58.63446	0(5000)
1	5	13	8	1.57300	58.64162	0(6000)
2	2	16	8	1.57099	58.72421	0(1100)
1	1	37	8	1.56782	58.85434	2(1400)
1	5	14	8	1.56084	59.14361	0(15000)
0	4	31	4	1.56078	59.14618	0(15000)
2	0	22	4	1.55759	59.27956	0(4000)
2	2	17	8	1.55622	59.33687	0(30000)

0	0	42	2	1.55608	59.34283	0(30000)
1	5	15	8	1.54809	59.67988	0(1000000)
0	6	0	2	1.54782	59.69128	0(2000000)
0	6	1	4	1.54739	59.70972	0(1400000)
0	6	2	4	1.54609	59.76501	0(500000)
1	3	32	8	1.54523	59.80181	0(700000)
0	6	3	4	1.54393	59.85710	0(400000)
0	2	40	4	1.54125	59.97175	0(3000000)
2	2	18	8	1.54100	59.98245	0(900000)
0	6	4	4	1.54093	59.98587	0(2000000)
0	6	5	4	1.53708	60.15119	0(2000000)
1	1	38	8	1.53505	60.23935	0(20000000)
1	5	16	8	1.53480	60.24991	0(20000000)
0	4	32	4	1.53348	60.30743	0(3000000)
0	6	6	4	1.53243	60.35287	0(1900000)
0	6	7	4	1.52698	60.59071	0(3000000)