

Table 1. Run conditions and fits to thermal diffusivity at elevated temperature

Name	Orientation and phase	L	D_{298}	D_{sat}	T_{sat}	Fit of $1/D$ vs T	Range	Structural transition temperatures; notes
		mm	mm ² /s	mm ² /s	K	s/mm ²	K	
CaTiO ₃ *	1† orth	0.80	1.336	0.71\$	>1700\$	$0.24041+0.0019518T-6.5443\times 10^{-7}T^2$	293-990	1200,1600 K Fit to first run
CaTiO ₃ *	2† orth	1.075	1.70	-	-	$0.10342+0.0019184T-7.6162\times 10^{-7}T^2$	293-990	1200 K, broke after run fit to first run
CaTiO ₃ *	3† orth	0.845	1.484	0.67\$	~1900\$	$0.22877+0.0017632T-6.3287\times 10^{-7}T^2$	293-990	1200,1600 K fit combines 2 runs
SrTiO ₃	cubic	1.87	4.279	-	-	$-0.033335+0.00097117T-2.0244\times 10^{-7}T^2$	293-900	Boule, first run, tan
SrTiO ₃	cubic	1.532	3.02	0.70	~1800	$-0.12178+0.0017177T-5.6751\times 10^{-7}T^2$	293-1300	Boule, third run, black
SrTiO ₃ §	cubic	0.991	3.49	-	-	$-0.051524+0.0012384T-3.4015\times 10^{-7}T^2$	293-950	Plate, first run
SrTiO ₃ §	cubic	0.985	3.05	0.71	~1800	$-0.057753+0.0014801T-5.8673\times 10^{-7}T^2$	293-840	Plate, third run, dark
SrTiO ₃ :Fe¶	cubic	0.505	3.65	0.73	~1800	$-0.037308+0.0011412T-2.6351\times 10^{-7}T^2$	293-1000	Plate, first run
SrTiO ₃ :Fe¶	cubic	0.505	2.91			$-0.027431+0.0014047T-5.0859\times 10^{-7}T^2$	293-800	Plate, second run, dark
BaTiO ₃	(001) tet	1.018	1.905			$-0.47329+0.0033704T$	293-390	390, 1100 K, premelting
BaTiO ₃	(100) tet	0.573	1.123			$0.45695+0.0014669T$ -	293-387	387 K
BaTiO ₃	cubic	both	1.73‡			$0.55807+0.001069T-2.8346\times 10^{-8}T^2$	390-900	1100 K, premelting
KNbO ₃	(110)? orth	0.93	1.958			$-0.15349+0.0017938T$	293-495	495 K
KNbO ₃	(110)? orth	2.035	1.693			$0.067158+0.0017477T$	293-495	495 K

KNbO ₃	tetragonal	0.93	‡				$-0.010169+0.0024206T-1.4292\times 10^{-6}T^2$	493-678	~685 K (run spacing wide)
KNbO ₃ #	cubic	0.93	‡				$0.73664+0.00032268T$	750-1050	Reduced ~1050 K
KTaO ₃	cubic	0.547	4.742				$-0.050405+0.00094559T-1.5221\times 10^{-7}T^2$	293-1200	~1600 K
LSAT*	cubic	0.516	1.615	0.71	~1300		$+0.34113+0.0010076T-1.6336\times 10^{-7}T^2$	293-1400	Black run same as colorless
LaAlO ₃	(100) rhomb	1.003	4.102				$-0.10664+0.0013367T-4.9895\times 10^{-7}T^2$	293-705	~750 K
LaAlO ₃	(110) rhomb	0.541	4.030				$-0.12222+0.0014092T-5.3988\times 10^{-7}T^2$	293-700	~750 K
LaAlO ₃	(001) rhomb	1.071	4.097						Boule, strong twinning
LaAlO ₃	(100) rhomb	1.055	4.008						Boule, slight twinning
LaAlO ₃	cubic	0.541, 1.003	4.32‡	0.96	1600- 1800		$-0.020134+0.00088093T-1.2173\times 10^{-7}T^2$	850-1620	Sample reddened
YAlO ₃	(100) ortho	0.465	3.913				$-0.17622+0.0016113T-2.9561\times 10^{-7}T^2$ &	293-1750	MTI sample
YAlO ₃	(100) ortho	0.985	3.758	-	-		$-0.22136+0.0017873T-4.2087\times 10^{-7}T^2$	293-1560	Non-stoichiometric sample from SMC
YAlO ₃ :Tm ¥	(001) ortho	0.975	2.907				$-0.15827+0.0018785T-5.1404\times 10^{-7}T^2$ @	293-1270	
NdGaO ₃	(100) ortho	0.523	1.93				$-0.1535+0.0025583T-7.6551\times 10^{-7}T^2$	293-1250	Plate turned blue ~1730 K, D similar to boule
NdGaO ₃	(010) ortho	0.945	1.84				$-0.25247+0.0030442T-11.069\times 10^{-7}T^2$	293-1250	Boule only
NdGaO ₃	(001) ortho	0.518, 0.734	2.02				$-0.14749+0.0023656T-5.7979\times 10^{-7}T^2$	293-1250	Fit to both boule and plate

Notes: All fits had residuals better than 0.99. Orth or ortho = orthorhombic ($Pbnm$) ; tet = tetragonal ($I4/mcm$); rhomb = rhombohedral ($R\bar{3}c$) structures.

* Chemical formulae obtained from electron microprobe analyses are $\text{Ca}_{1.01}\text{Mn}_{0.001}\text{Fe}_{0.007}\text{Ti}_{0.99}\text{O}_3$ and $\text{La}_{0.29}\text{Sr}_{0.67}\text{Al}_{0.65}\text{Ta}_{0.35}\text{O}_3$.

† The sample is twinned. Three perpendicular cuts were examined in order to provide an “average” D . Section No. 3 provided reproducible data. Both runs were fit.

‡ Room temperature values obtained by extrapolating the fit made to the higher temperature data. For BaTiO_3 , the extrapolation is over a short temperature range and gives D_{298} of the cubic polymorph that is higher than that the tetragonal, as is seen at the transition temperature. Extrapolations for KNbO_3 are not reported because the small temperature ranges of the polymorphs do not constrain terms beyond linear and thus do not provide reliable values. The fit for the cubic polymorph of LaAlO_3 should be considered a lower limit, given that the extrapolation is made over 500 K.

§ Appears to be initially partially reduced or non-stoichiometric, see text.

¶ Doped with 0.05 atom % Fe^{3+}

¥ Doped with 5.3 atom % Tm^{3+}

Trend for cubic perovskite was taken from the thin piece KNbO_3 which was heated to high T in one run. A run on a thicker sample was terminated within tetragonal field (due to a power failure). As the sample was highly fractured, probably twinned during cooling, the results are questionable and are not reported.

\$ Pertains to cubic phase of CaTiO_3 .

& From combining our data with D of Aggarwal et al.²⁴, the fit for undoped (100) from 200 to 1750 K is $1/D = -0.25271 + 0.0019025T - 6.111 \times 10^{-7} T^2 + 1.0144 \times 10^{-10} T^3$. We have assumed that their orientations were interchanged, see Table 2 and the text. The sample from SMC only differs from D for the MTI sample near 298 K.

@ From combining our data on the (001) Tm doped sample with D from Aggarwal et al.²⁴ for Yb doped YAlO_3 , the fit for (001) sections with ~5 atom % dopant from 150 to 1250 K is $1/D = -0.17027 + 0.0019133T - 5.3556 \times 10^{-7} T^2$. These ions differ little in physical properties and are considered equivalent.

Table 2. Physical properties at 298 K and transition temperatures from the literature with comparison to present results

Sample	Density g/cm ³	C_p J/g-K	Mass g/mol	$T_{\text{ortho-tet}}$ K	$T_{\text{tet-cubic}}$ K	T_{melt} K	Ref.	D_{298} mm ² s ⁻¹	D_{298} mm ² s ⁻¹	Method	Temp K	Ref.
CaTiO ₃	4.1	0.721	135.94	~1384	~1520	2250	41,42,54	1.5 ave	-	-	-	-
SrTiO ₃	5.17	0.536	183.48	-	110	2353	51	4.28	4.01	LFA†	>298	23
BaTiO ₃	6.06	0.527	233.21	278	408	1895	26	1.91 c	1.25 c	2 contacts	<298	23
								1.12 ⊥c	1.65 ⊥c	2 contacts	<298	23
KNbO ₃	4.62	~0.57	179.99	498	707	1050	26	2.0 ⊥c?	4.18-2.87 b	2 contacts	<298	23
KTaO ₃	7.01	0.375	268.08	-	-	1625	25	4.74	3.27	LFA†‡	>298	25
									6.66	2 contacts	<298	26
LSAT	6.64	0.35	201.38	-	~150	2143	47	1.61	1.9±0.1	LFA†	=298	22
	6.74								1.33±0.13	contact	=298	44
LaAlO ₃	6.70	0.427	213.88	-	806*	2350	45	4.05 ave	4.87 c	1 contact	<298	45
	6.51			-					4.5±0.5 ?	2 contacts	=298	44
	6.52			-					4.0±0.3 a	2 contacts	<298	46
				-					3.2 a	2, steady st.	<298	43
YAlO ₃	5.35	0.557	163.87	-	-	2143	24	3.91 a	4.5 a?§	lfa Au coat	<298	24
				-	3.9 b?§			lfa Au coat	<298	24		
				-	3.3 c?§			lfa Au coat	<298	24		
YAlO ₃ :X	5.35	0.557	163.87	-	-	2143	24	-	2.6 a	lfa Au coat	<298	24
				-	2.3 b			lfa Au coat	<298	24		
				-	2.91 c			lfa Au coat	<298	24		

NdGaO ₃	7.66	0.404	261.96	-	-	1870	45	1.93 a	2.0 c ⊥ c	2 contacts	=298	44
								1.84 b	2.3 (110)	1 contact	<298	45
								2.02 c				

Notes: The *Pbnm* convention is used for orthorhombic samples. Results from Aggarwal et al.²⁴ were translated from their reported *Pnma* convention.

*Rhombohedral to cubic transition.

†Analysis did not account for radiative transfer.

‡An overly thick sample was used.

¶Our sample of YAlO₃ ||**b** was doped with 5.3 atom % Tm, whereas that of Aggarwal et al.²⁴ had 5 atom% Yb.

§Based on the order $D_c > D_a > D_b$ for NdGaO₃ and doped YAlO₃, which is consistent with the lattice parameters for the primitive cell (see text), and that our two different samples of YAlO₃ both provided $D_a = 3.9 \text{ mm}^2\text{s}^{-1}$, we believe that the orientations for pure YAlO₃ for the previous study²⁴ were interchanged. Heat flow parallel to the **a**-axis should yield $3.9 \text{ mm}^2\text{s}^{-1}$; the **b**-axis should yield $3.3 \text{ mm}^2\text{s}^{-1}$, and the **c**-axis should yield $4.5 \text{ mm}^2\text{s}^{-1}$.