of Equation 7 of [2], for a bimodal distribution in which there was little or no overlap between the large and small size range flaw populations.

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X-ray characterization of $SrCeO_3$ and $BaCeO_3$

The compounds $SrCeO_3$ and $BaCeO_3$ have been examined by numerous authors in order to determine their crystal structures. Both compounds exhibit non-ideal perovskite-type crystal structures; with regard to their symmetry, however, a great deal of the data reported in the literature are often in disagreement.

$SrCeO_3$ has been assigned, with varying lattice parameters, a cubic cell [1, 2], a tetragonal cell [2, 3], an orthorhombic cell [4–7] and a monoclinic cell [8–10]. According to Preda and Dinescu [2], $SrCeO_3$ undergoes a phase transition from a high-temperature cubic structure, obtainable by quenching, to a low-temperature tetragonal structure, obtainable by slow cooling.

$BaCeO_3$ has been assigned, with varying lattice parameters, a cubic cell [1–5, 11, 12], a tetragonal cell [2], an orthorhombic cell [6] and a monoclinic cell [9, 10]. For $BaCeO_3$, too, Preda and Dinescu [2] have found evidence of a phase transition from a high-temperature cubic structure, obtainable by rapid cooling, to a low-temperature tetragonal structure, obtainable by slow cooling.

Because of their interesting electrical characteristics, which have been pointed out by Longo *et al.* [13], $SrCeO_3$ and $BaCeO_3$ appear to be suitable materials for use as high-temperature semiconductors; therefore, the present investigation was undertaken in order to determine the crystal structures of the two cerates under different operating conditions and to verify the existence of the phase transition reported by Preda and Dinescu [2].

The raw materials used were CeO_2 (99.9% pure) and reagent grade $SrCO_3$ and $BaCO_3$. To prepare the stoichiometric compounds in the mole ratio of 1 : 1, the starting materials were weighed, mixed and homogenized by hand-mixing in agate mortars for 4 h, pressed into discs and air-fired at 1400° C for long time periods to ensure the completion of the reactions; equilibrium was considered to have been attained when the X-ray diffraction patterns of specimens subjected to successive heating and cooling treatments showed no further change.

The specimens were subjected to different cooling treatments: namely, some of them were quenched in water at 20° C, some were cooled in air, some were allowed to cool in the oven, and some were annealed at a temperature of 450° C for

TABLE I Crystal data of $SrCeO_3$

Parameter	Value
a	5.997 ± 0.002 Å
b	12.308 ± 0.004 Å
c	8.615 ± 0.003 Å
V	635.88 Å^3
FW	275.74
Z	8
δ_{calc}	5.76 g cm^{-3}
δ_{exp}	5.68 g cm^{-3}

V = volume, FW = formula weight, Z = number of formula weights per unit cell, δ_{calc} = calculated density and δ_{exp} = experimental density.

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TABLE II X-ray powder diffraction data of $SrCeO_3$ at 20° C

$h\ k\ l$	d_{calc}	d_{obs}	I_{obs}
1 10	5.391	5.37	M
0 02	4.307	4.301	MS
1 20	4.295		
1 21	3.844	3.850	W
0 40	3.077	3.079	S
1 22	3.041	3.040	VS
2 00	2.999	3.004	S
0 32	2.971	2.969	MS
1 03	2.590	2.587	W
1 23	2.387	2.384	W
1 50	2.277	2.276	W
2 40	2.147	2.146	S
0 14	2.122	2.125	M
2 41	2.084	2.087	W
1 60	1.941	1.941	W
1 24	1.925	1.922	M
3 11	1.923		
2 42	1.922		
1 61	1.894	1.894	M
1 62	1.770	1.770	S
0 44	1.764	1.763	MS
3 31	1.759		
2 52	1.740	1.742	S
3 22	1.739		
0 71	1.723	1.722	M
2 43	1.720		
3 40	1.677	1.677	VW
2 34	1.609	1.606	W
1 63	1.608		
0 80	1.538	1.537	W
1 35	1.536		
2 70	1.517	1.518	M
0 45	1.503	1.502	M
4 00	1.500		
4 21	1.436	1.438	W
0 06	1.436		
2 80	1.369	1.368	W
3 53	1.365		
3 62	1.359	1.359	S
2 81	1.352	1.350	MW
0 91	1.351		
4 40	1.348		
3 05	1.305	1.305	VW
3 71	1.305		
2 82	1.305		
2 16	1.288	1.287	VW
4 42	1.286		
0 84	1.252	1.251	VW
2 91	1.232	1.232	M
0100	1.231		
0 75	1.231		
4 04	1.231		
3 64	1.192	1.191	W
1102	1.161	1.162	VW
3 16	1.161		
1 66	1.154	1.152	M
3 55	1.153		
5 30	1.151		
5 12	1.150		
2 56	1.146	1.144	M
0 47	1.143		
4 44	1.143		
2 93	1.142		

Intensities: VS = very strong, S = strong, MS = medium strong, M = medium, MW = medium weak, W = weak, VW = very weak.

a period of two months. Such a procedure was followed in order to verify that the allotropic transformation reported by Preda and Dinescu [2], occurred in the two metacerates examined.

Debye–Scherrer powder diffraction patterns were obtained in a camera, 114.6 mm in diameter using CuKα radiation. Reflections were recorded by means of a goniometer and a Guinier–de Wolff camera using CuKα radiation. Intensities were determined by a scintillation counter in conjunction with a pulse-height analyser at a scanning rate of $1°\ 2\theta\ \mathrm{min}^{-1}$. Calibration of X-ray patterns was carried out using $Pb(NO_3)_2$ as an internal standard. Density measurements were made using the picnometric method.

The diffraction patterns of the specimens quenched in water at 20° C were identical to those of the specimens cooled in air or allowed to cool in the oven or annealed at 450° C. No evidence was

TABLE III Crystal data of $BaCeO_3$

Parameter	Value
a	6.212 ± 0.002 Å
b	
c	8.804 ± 0.004 Å
V	339.69 Å^3
FW	325.45
Z	4
δ_{calc}	6.36 g cm^{-3}
δ_{exp}	6.29 g cm^{-3}
sg (prob.)	92

V = volume, FW = formula weight, Z = number of formula weights per unit cell, δ_{calc} = calculated density, δ_{exp} = experimental density and sg (prob.) = space group (probable).

TABLE IV X-ray powder diffraction data of $BaCeO_3$ at 20° C

hkl	d_{calc}	d_{obs}	I_{obs}
112	3.109	3.105	VVS
200	3.106		
103	2.653	2.650	VW
211	2.649		
202	2.538	2.540	VW
004	2.201	2.204	S
220	2.196	2.194	S
221	2.131	2.128	VW
222	1.965	1.961	VW
310	1.964		
311	1.917	1.916	VW
204	1.796	1.801	VS
312	1.794	1.792	VS
224	1.555	1.556	S
400	1.553	1.552	S
116	1.392	1.390	S
332	1.389	1.388	S
420	1.389		
404	1.269	1.269	M
316	1.176	1.177	S
424	1.175	1.173	S
512	1.174		
513	1.125	1.123	VVW
008	1.100	1.100	W
440	1.098	1.097	W
208	1.037		
336	1.036	1.038	MS
600	1.035	1.036	MS
532	1.035		

Intensities: VVS = very very strong, VS = very strong, S = strong, MS = medium strong, M = medium, W = weak, VW = very weak, VVW = very very weak.

therefore found of the allotropic transformation previously reported [2] which is thus excluded by the present writers.

The compound $SrCeO_3$ was indexed according to orthorhombic symmetry. The least squares refined lattice parameters are $a = 5.997 \pm 0.002$ Å, $b = 12.308 \pm 0.004$ Å and $c = 8.615 \pm 0.003$ Å at room temperature. Crystal data of the phase are summarized in Table I; spacing values are reported in Table II.

The X-ray diffraction pattern of $BaCeO_3$ was indexed on the basis of a tetragonal unit cell. The least squares refined lattice parameters are $a = b = 6.212 \pm 0.002$ Å and $c = 8.804 \pm 0.004$ Å at room temperature. Crystal data of the phase are summarized in Table III; spacing values are reported in Table IV.

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