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E. N. Maslen, V. A. Streltsov, N. R. Streltsova, N. Ishizawa and Y. Satow

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Material for deposit

Lists of structure factors for all of 5 data sets and figures of deformation density sections in (01$\bar{1}$0) plane through O and two Al atoms for data sets 1,3,4,5 and 3 scaled on data set 2 with the extinction corrections evaluated by minimizing differences between equivalent reflection intensities and with the extinction parameter included in the structure refinement.

Synchrotron X-ray Study of the Electron Density in α-Al_2O_3

By E. N. Maslen, V. A. Streltsov* and N. R. Streltsova,
Crystallography Centre, University of Western Australia, Nedlands, 6009, Australia
N. Ishizawa,
Research Laboratory of Engineering Materials, Tokyo Institute of Technology, 4259 Nagatsuta, Midori-Ku, Yokohama 227, Japan
Y. Satow
Faculty of Pharmaceutical Sciences, University of Tokyo, Hongo 7-3-1, Bunkyo-ku, Tokyo 113, Japan

Abstract

Structure factors for corundum α-Al_2O_3, have been measured using 0.7 Å and 0.9 Å synchrotron radiation as well as Mo $K\alpha$ (λ = 0.71069 Å) radiation. The stronger structure factors from two sets of synchrotron data and three sets of Mo Ka tube data for two small crystals are remarkably consistent. In analysing those data, extinction corrections evaluated by minimizing differences between equivalent reflection intensities were compared with those from the more common procedure of least squares determination of the extinction parameters as a part of the structure refinement. Difference electron densities evaluated with extinction corrections from equivalent reflection intensities are more consistent than those which optimize $|F_o|$ v $|F_c|$ agreement. Approximate symmetry in the concordant densities is related more closely to the Al-Al geometry than to nearest neighbour Al-O interactions. Space group $R\bar{3}c$, hexagonal, M_r = 101.96, a = 4.7540 (5) Å, c = 12.9820 (6) Å, V = 254.09 (6) Å^3, Z = 6, D_x = 3.997 Mg m^{-3}, $\mu_{0.9}$ = 2.361, $\mu_{0.7}$ = 1.097, $\mu_{Mo\ K\alpha}$ = 1.139 mm^{-1}, $F(000)$ = 300, T = 293 K, R = 0.024, wR = 0.030, S = 4.84 for the unique 0.7Å synchrotron reflection data.

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* Author to whom correspondence should be addressed.

Data set 1

h	k	l	Fo	σ(Fo)
0	-2	2	13.742	.300
0	-4	4	37.861	.371
0	-6	6	9.272	.784
-1	9	-7	14.000	.509
-1	8	-6	24.064	.424
-1	6	-4	44.012	.324
-1	5	-3	24.414	.291
-1	4	-2	32.177	.239
-1	3	-1	18.787	.215
-1	2	0	58.448	.218
-1	0	2	48.667	.184
-1	-1	3	77.718	.176
-1	-2	4	76.093	.208
-1	-3	5	7.051	.418
-1	-4	6	52.600	.291
-1	-5	7	14.709	.393
-1	-6	8	18.915	.423
-1	-7	9	9.599	.623
-2	8	-4	32.122	.397
-2	7	-3	14.302	.436
-2	6	-2	12.400	.389
-2	5	-1	12.162	.321
-2	4	0	54.437	.321
-2	0	4	89.439	.293
-2	-1	5	15.403	.244
-2	-2	6	70.808	.247
-2	-3	7	10.630	.373
-2	-4	8	16.148	.382
-2	-5	9	13.128	.485
-2	-6	10	15.958	.479
-3	6	0	72.235	.419
-3	0	6	14.643	.359
-3	-1	7	8.350	.357
-3	-2	8	12.731	.347
-3	-4	10	44.253	.370
-3	-5	11	9.737	1.501
-3	-6	12	12.251	.497
-4	10	-2	15.513	.479
-4	9	-1	13.342	.484
-4	8	0	25.666	.558
-4	0	8	38.716	.402
-4	-1	9	21.522	.342
-4	-2	10	37.766	.341
-4	-5	13	10.738	.560
-5	10	0	15.388	.638
-5	0	10	31.493	.485
-5	-1	11	14.022	.415
-6	0	12	19.756	.583
-6	-2	14	27.029	.420
0	7	-4	8.387	.816
0	3	0	127.477	.436
0	-1	4	79.547	.236
0	-3	6	33.685	.382
0	-5	8	10.204	.634
0	-7	10	40.534	.566
-1	9	-4	24.707	.436
-1	8	-3	10.717	.557
-1	7	-2	16.522	.427
-1	6	-1	15.584	.371
-1	5	0	45.122	.277
-1	4	1	9.081	.326
-1	3	2	20.867	.209
-1	-1	6	95.588	.516
-1	-2	7	12.822	.267
-1	-3	8	34.144	.269
-1	-4	9	21.354	.333
-1	-5	10	29.132	.361
-2	8	-1	13.111	.495
-2	7	0	28.019	.360
-2	6	1	12.706	.369
-2	5	2	7.111	.396
-2	4	3	36.081	.234
-2	-1	8	26.992	.240
-2	-2	9	27.509	.282
-2	-3	10	37.467	.310
-2	-4	11	9.639	.515
-2	-6	13	11.053	.600
-3	9	0	34.653	.406
-3	7	2	25.860	.358
-3	5	4	61.133	.270
-3	-1	10	61.485	.281
-3	-2	11	9.476	.426
-3	-3	12	24.503	.373
-3	-5	14	26.642	.423
-4	8	3	12.559	.503
-4	7	4	17.398	.397
-4	6	5	11.274	.407
-4	-2	13	9.914	.534
-4	-3	14	13.933	.491
-4	-4	15	10.282	.608
-5	9	4	25.565	.424
-5	7	6	35.249	.364
-5	-1	14	34.034	.376
-5	-2	15	11.597	.520
-5	-3	16	20.659	.447
-6	8	7	13.239	.502
-6	-1	16	9.357	.635
0	6	0	58.092	.469
0	4	2	38.969	.357
0	0	6	18.665	.441
0	-2	8	25.221	.313
0	-4	10	63.674	.419
0	-6	12	20.446	.576
-1	9	-1	13.818	.517
-1	8	0	22.008	.426
-1	5	3	24.719	.286
-1	4	4	50.177	.243
-1	0	8	44.239	.277
-1	-1	9	43.673	.222
-1	-2	10	61.541	.254
-1	-5	13	13.173	.479
-1	-6	14	16.750	.481
-2	7	3	13.771	.430
-2	6	4	40.363	.312
-2	5	5	10.754	.378
-2	0	10	62.125	.336
-2	-1	11	9.477	.358
-2	-2	12	7.908	.434
-2	-4	14	29.420	.382
-2	-5	15	10.893	.578
-2	-6	16	20.894	.430
-3	8	4	33.810	.383
-3	6	6	12.715	.381
-3	0	12	38.872	.406
-3	-1	13	7.098	.476
-3	-2	14	41.632	.345

-4	9	5	12.981	.528
-4	8	6	26.858	.400
-4	0	14	25.778	.498
-4	-1	15	16.483	.437
-4	-2	16	19.264	.439
-5	10	6	20.614	.445
-5	9	7	11.081	.585
-5	0	16	27.571	.570
-5	-1	17	11.153	.546
-6	0	18	25.631	.601
0	7	2	25.796	.562
0	5	4	52.770	.421
0	-1	10	79.558	.315
0	-3	12	38.672	.406
0	-5	14	36.919	.512
-1	8	3	10.560	.593
-1	7	4	21.222	.405
-1	6	5	14.746	.381
-1	5	6	52.493	.292
-1	-1	12	9.756	.353
-1	-2	13	9.412	.388
-1	-3	14	33.344	.330
-1	-4	15	17.664	.417
-1	-5	16	24.572	.409
-2	9	4	19.305	.478
-2	8	5	13.434	.501
-2	7	6	36.061	.359
-2	6	7	12.390	.408
-2	-1	14	47.402	.298
-2	-2	15	21.138	.357
-2	-3	16	29.189	.372
-3	9	6	8.955	.598
-3	7	8	27.865	.375
-3	-1	16	18.752	.381
-3	-3	18	29.969	.396
-4	8	9	12.206	.514
-4	-3	20	28.176	.428
-5	9	10	17.384	.452
-5	-1	20	15.687	.493
0	8	4	24.769	.615
0	6	6	11.178	.648
0	0	12	53.556	.587
0	-2	14	53.445	.402
0	-4	16	12.503	.593
0	-6	18	24.627	.602
-1	9	5	14.316	.469
-1	8	6	23.847	.422
-1	6	8	8.561	.548
-1	0	14	49.876	.380
-1	-1	15	26.689	.303
-1	-2	16	30.934	.332
-1	-5	19	10.063	.640
-2	7	9	12.416	.489
-2	0	16	37.226	.427
-2	-4	20	21.587	.426
-3	8	10	17.545	.475
-3	0	18	40.280	.509
-3	-2	20	19.611	.428
-4	9	11	12.021	.509
-4	0	20	35.383	.563
-4	-1	21	14.544	.471
0	7	8	28.089	.568
0	-1	16	30.007	.430
0	-3	18	41.470	.501
0	-5	20	17.838	.617
-1	8	9	9.029	.673
-1	7	10	34.745	.382
-1	-1	18	9.565	.432
-1	-3	20	32.382	.392
-1	-4	21	14.185	.496
-2	9	10	19.689	.440
-2	8	11	11.584	.587
-2	-1	20	28.513	.382
-2	-2	21	16.111	.485
-3	9	12	12.382	.517
-4	-1	24	25.509	.415
0	8	10	15.232	.635
0	0	18	50.769	.768
0	-2	20	28.243	.543
-1	0	20	37.214	.482
-1	-1	21	20.106	.415
-1	-4	24	24.941	.417
-2	-2	24	30.550	.399
-1	-1	24	34.209	.395
-2	-1	26	12.798	.517
0	-2	26	15.937	.673
-1	0	26	10.551	.874
-1	-1	27	15.679	.463

Data set 2

h	k	l	Fo	σ(Fo)
0	-2	2	13.841	.140
0	-4	4	38.162	.196
0	-6	6	11.085	.229
-1	8	-6	24.520	.172
-1	7	-5	5.818	.168
-1	6	-4	44.600	.158
-1	5	-3	25.255	.145
-1	4	-2	32.209	.130
-1	3	-1	18.859	.111
-1	2	0	56.753	.522
-1	0	2	46.544	.116
-1	-1	3	74.698	.419
-1	-2	4	74.991	.325
-1	-3	5	7.679	.133
-1	-4	6	53.322	.150
-1	-5	7	14.623	.160
-1	-6	8	18.738	.169
-1	-7	9	9.828	.173
-2	8	-4	32.946	.170
-2	7	-3	14.111	.162
-2	6	-2	13.291	.153
-2	5	-1	12.004	.140
-2	4	0	54.411	.182
-2	0	4	87.272	.195
-2	-1	5	15.603	.119
-2	-2	6	70.773	.139
-2	-3	7	10.904	.323
-2	-4	8	16.635	.159
-2	-5	9	13.078	.167
-2	-6	10	16.412	.172
-3	9	-3	2.221	.184
-3	8	-2	1.189	.195
-3	7	-1	2.850	.165
-3	6	0	72.750	.219
-3	0	6	14.397	.178
-3	-1	7	7.989	.137
-3	-2	8	12.704	.148

-3	-3	9	.985	.218
-3	-4	10	44.863	.168
-3	-5	11	6.913	.172
-4	9	-1	12.801	.170
-4	8	0	26.336	.236
-4	0	8	39.139	.206
-4	-1	9	21.676	.153
-4	-2	10	37.743	.162
-4	-3	11	1.671	.190
-4	-4	12	.927	.242
-5	0	10	31.929	.224
-5	-1	11	13.313	.164
-5	-2	12	4.579	.169
-5	-3	13	6.658	.172
-6	0	12	20.533	.237
-6	-1	13	5.640	.171
-7	0	14	6.291	.242
0	7	-4	8.537	.237
0	5	-2	5.055	.213
0	3	0	123.056	.446
0	-1	4	73.352	.810
0	-3	6	13.818	.179
0	-5	8	9.493	.220
0	-7	10	42.087	.244
-1	8	-3	10.387	.171
-1	7	-2	16.584	.164
-1	6	-1	16.300	.155
-1	5	0	46.161	.144
-1	4	1	8.827	.129
-1	3	2	21.050	.112
-1	-1	6	92.811	.559
-1	-2	7	12.330	.125
-1	-3	8	34.441	.141
-1	-4	9	21.434	.153
-1	-5	10	29.339	.164
-1	-6	11	4.539	.171
-2	9	-2	5.950	.172
-2	8	-1	13.311	.168
-2	7	0	28.237	.161
-2	6	1	12.265	.151
-2	5	2	6.637	.140
-2	4	3	36.530	.129
-2	-1	8	27.648	.128
-2	-2	9	28.370	.141
-2	-3	10	38.331	.153
-2	-4	11	9.896	.162
-2	-5	12	4.366	.171
-3	9	0	34.545	.172
-3	8	1	7.887	.167
-3	7	2	25.722	.160
-3	6	3	1.316	.181
-3	5	4	60.891	.146
-3	-1	10	62.001	.148
-3	-2	11	9.154	.154
-3	-3	12	24.449	.163
-3	-4	13	2.491	.176
-3	-5	14	27.087	.172
-4	9	2	1.799	.172
-4	8	3	13.066	.167
-4	7	4	17.753	.161
-4	6	5	11.915	.154
-4	-1	12	4.571	.160
-4	-2	13	10.248	.165
-4	-3	14	12.918	.170
-5	9	4	25.920	.171
-5	8	5	7.828	.168
-5	7	6	35.970	.165
-5	-1	14	33.454	.168
-5	-2	15	11.337	.170
-6	9	6	8.000	.172
-6	8	7	13.072	.171
-6	-1	16	9.716	.171
0	8	-2	-.069	.622
0	6	0	59.106	.229
0	4	2	37.991	.193
0	0	6	18.433	.230
0	-2	8	25.324	.172
0	-4	10	63.861	.217
0	-6	12	20.504	.237
-1	8	0	21.750	.170
-1	7	1	5.961	.164
-1	6	2	4.677	.156
-1	5	3	25.334	.144
-1	4	4	50.603	.134
-1	0	8	43.526	.159
-1	-1	9	43.767	.124
-1	-2	10	61.612	.139
-1	-3	11	5.436	.148
-1	-4	12	4.643	.156
-1	-5	13	13.003	.166
-1	-6	14	17.525	.171
-2	9	1	7.659	.172
-2	8	2	1.092	.231
-2	7	3	14.200	.162
-2	6	4	40.131	.155
-2	5	5	11.680	.143
-2	0	10	62.510	.189
-2	-1	11	9.774	.139
-2	-2	12	6.835	.150
-2	-3	13	8.273	.158
-2	-4	14	29.585	.167
-2	-5	15	11.523	.171
-3	9	3	2.388	.174
-3	8	4	33.933	.168
-3	7	5	20.546	.164
-3	6	6	12.665	.155
-3	0	12	39.478	.206
-3	-1	13	5.941	.153
-3	-2	14	41.355	.162
-3	-3	15	1.229	.209
-3	-4	16	5.027	.172
-4	9	5	12.164	.171
-4	8	6	27.517	.169
-4	7	7	2.798	.170
-4	0	14	25.255	.224
-4	-1	15	17.512	.164
-4	-2	16	18.984	.169
-4	-3	17	1.345	.216
-5	9	7	12.174	.172
-5	8	8	4.226	.170
-5	0	16	27.849	.236
-5	-1	17	11.162	.169
-6	0	18	24.749	.241
0	7	2	26.439	.235
0	5	4	52.926	.214
0	-1	10	78.836	.183
0	-3	12	39.334	.205
0	-5	14	37.263	.232

-1	8	3	10.320	.169
-1	7	4	21.840	.164
-1	6	5	14.937	.156
-1	5	6	53.270	.149
-1	-1	12	9.534	.135
-1	-2	13	8.768	.145
-1	-3	14	33.481	.156
-1	-4	15	17.647	.163
-1	-5	16	23.725	.169
-2	9	4	19.832	.170
-2	8	5	13.330	.168
-2	7	6	35.885	.164
-2	6	7	11.651	.156
-2	-1	14	47.726	.149
-2	-2	15	21.079	.156
-2	-3	16	29.505	.164
-2	-4	17	8.133	.168
-3	9	6	8.197	.170
-3	8	7	7.535	.168
-3	7	8	28.013	.164
-3	-1	16	18.778	.159
-3	-2	17	7.354	.165
-3	-3	18	29.267	.170
-4	9	8	4.468	.172
-4	8	9	12.137	.169
-4	-1	18	6.995	.167
-4	-2	19	8.552	.170
0	8	4	26.231	.241
0	6	6	10.122	.228
0	0	12	53.349	.322
0	-2	14	54.410	.208
0	-4	16	12.013	.228
0	-6	18	25.737	.242
-1	8	6	24.167	.170
-1	7	7	6.193	.166
-1	6	8	9.125	.160
-1	0	14	49.657	.200
-1	-1	15	26.885	.147
-1	-2	16	30.951	.155
-1	-3	17	4.150	.162
-1	-4	18	6.210	.168
-1	-5	19	10.527	.171
-2	8	8	2.436	.183
-2	7	9	12.679	.166
-2	0	16	35.830	.215
-2	-1	17	6.842	.157
-2	-2	18	7.020	.163
-2	-3	19	7.040	.168
-2	-4	20	21.393	.171
-3	8	10	17.641	.171
-3	0	18	42.208	.230
-3	-1	19	4.434	.168
-3	-2	20	19.302	.170
-4	0	20	35.519	.239
-4	-1	21	14.361	.171
[illegible]		0	28.111	.240
0	-1	16	30.461	.209
0	-3	18	41.584	.230
0	-5	20	16.748	.240
-1	8	9	9.263	.171
-1	7	10	34.861	.169
-1	-1	18	8.517	.156
-1	-2	19	6.664	.163
-1	-3	20	32.171	.168
-1	-4	21	14.060	.170
-2	8	11	12.736	.171
-2	-1	20	28.621	.165
-2	-2	21	16.491	.169
-2	-3	22	6.178	.170
-3	-1	22	5.446	.169
0	0	18	50.561	.381
0	-2	20	28.891	.231
0	-4	22	9.454	.240
-1	0	20	36.629	.229
-1	-1	21	19.743	.165
-1	-2	22	1.344	.222
-1	-3	23	2.858	.179
-2	0	22	4.315	.237
-2	-1	23	5.039	.171
-3	0	24	4.307	.243
0	-1	22	3.144	.240
0	-3	24	3.963	.240
-1	-1	24	34.396	.170
0	0	24	4.900	.399

Data set 3

h	k	l	Fo	σ(Fo)
0	-2	2	13.641	.035
0	-4	4	37.285	.245
0	-6	6	10.463	.052
-1	8	-6	23.945	.036
-1	7	-5	5.551	.037
-1	6	-4	43.020	.182
-1	5	-3	24.783	.098
-1	4	-2	31.378	.162
-1	3	-1	18.252	.077
-1	2	0	54.510	.884
-1	0	2	44.703	.152
-1	-1	3	70.719	.591
-1	-2	4	71.503	.455
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Data set 4

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Data set 5

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4	8	3	12.754	.381
4	7	4	17.341	.313
4	6	5	11.572	.324
4	-1	12	5.586	.561
4	-2	13	10.055	.402
4	-3	14	13.193	.402
5	9	4	15.713	.340
5	8	5	8.721	.450
5	7	6	36.338	.292
5	-1	14	32.953	.319
5	-2	15	11.515	.413
6	9	6	7.701	.559
6	8	7	13.525	.390
0	6	0	57.271	.386

0	4	2	37.128	.295
0	0	6	19.200	.366
0	-2	8	25.147	.262
0	-4	10	63.827	.346
0	-6	12	19.628	.483
-1	8	0	22.025	.339
-1	7	1	5.402	.623
-1	6	2	4.506	.561
-1	5	3	24.849	.235
-1	4	4	49.864	.200
-1	0	8	44.510	.231
-1	-1	9	44.089	.185
-1	-2	10	61.987	.212
-1	-3	11	5.220	.444
-1	-4	12	5.545	.489
-1	-5	13	12.905	.361
-1	-6	14	18.308	.587
-2	9	1	7.920	.556
-2	7	3	13.889	.336
-2	6	4	39.734	.257
-2	5	5	11.635	.273
-2	0	10	62.668	.285
-2	-1	11	9.766	.275
-2	-2	12	6.146	.425
-2	-3	13	8.775	.377
-2	-4	14	29.810	.313
-2	-5	15	12.094	.686
-3	8	4	33.281	.317
-3	6	6	12.540	.308
-3	0	12	38.575	.336
-3	-1	13	6.040	.440
-3	-2	14	40.562	.287
-4	9	5	12.053	.440
-4	8	6	27.489	.318
-4	0	14	25.090	.398
-4	-1	15	16.976	.343
-4	-2	16	19.324	.341
-5	9	7	12.518	.411
-5	0	16	27.964	.452
-5	-1	17	10.279	.479
0	7	2	27.294	.434
0	5	4	52.201	.347
0	-1	10	80.930	.296
0	-3	12	38.596	.340
0	-5	14	36.801	.428
-1	8	3	9.981	.447
-1	7	4	21.506	.320
-1	6	5	14.739	.306
-1	5	6	52.409	.238
-1	-1	12	9.169	.293
-1	-2	13	8.914	.316
-1	-3	14	33.066	.271
-1	-4	15	17.689	.331
-1	-5	16	23.192	.609
-2	8	5	13.255	.385
-2	7	6	30.059	.291
-2	6	7	12.183	.316
-2	-1	14	48.158	.245
-2	-2	15	20.964	.298
-2	-3	16	29.237	.310
-2	-4	17	8.344	.884
-3	9	6	7.678	.566
-3	8	7	7.527	.527
-3	7	8	28.015	.303
-3	-1	16	19.056	.309
-3	-2	17	6.418	.653
-3	-3	18	29.844	.575
-4	8	9	11.773	.423
-4	-1	18	7.058	.523
-4	-2	19	8.941	.879
0	8	4	26.775	.487
0	6	6	10.826	.540
0	0	12	53.450	.492
0	-2	14	54.179	.332
0	-4	16	12.747	.519
-1	8	6	23.626	.338
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-1	6	8	9.571	.375
-1	0	14	50.211	.320
-1	-1	15	27.181	.253
-1	-2	16	31.329	.271
-1	-4	18	6.560	.944
-1	-5	19	11.390	.746
-2	7	9	13.139	.380
-2	0	16	36.444	.367
-2	-1	17	6.806	.454
-2	-2	18	7.453	.455
-2	-3	19	8.177	.787
-3	8	10	18.618	.357
-3	0	18	40.651	.418
-3	-2	20	19.322	.593
-4	0	20	35.013	.471
-4	-1	21	14.263	.690
0	7	8	27.528	.464
0	-1	16	30.067	.354
0	-3	18	41.864	.414
0	-5	20	16.711	.967
-1	8	9	9.669	.472
-1	7	10	34.537	.318
-1	-1	18	8.694	.402
-1	-2	19	6.768	.512
-1	-3	20	32.618	.559
-1	-4	21	15.464	.653
-2	8	11	12.009	.446
-2	-1	20	29.070	.311
-2	-2	21	16.760	.626
0	0	18	50.789	.654
0	-2	20	29.410	.418
0	-4	22	8.987	1.255
-1	0	20	36.634	.416
-1	-1	21	19.537	.339
0	-1	22	5.561	.681
0	-3	24	5.259	1.442
-1	-1	24	33.608	.583
0	0	24	7.639	1.038

Figure legends

Fig. 1. Δr for α-Al_2O_3 in the $(01\bar{1}0)$ plane through two Al and three O atoms with two O atoms deviating from the plane by 0.11 Å shown in italics. Extinction corrections were evaluated by minimizing differences between equivalent reflection intensities. (*a*) data set 1, (*b*) data set 3, (*c*) data set 4, (*d*) data set 5. Map borders 5.1 by 5.9 Å. Contour interval 0.1 $eÅ^{-3}$, positive, negative contours - solid, short dashes respectively.

Fig. 2. Δr for α-Al_2O_3 in the plane as Fig. 1.Extinction corrections were determined as part of the least squares structure refinement. (*a*) data set 1, (*b*) data set 3, (*c*) data set 4, (*d*) data set 5. Map borders and contour interval as for Fig. 1.

Fig 3. Δr for α-Al_2O_3 in the $(01\bar{1}0)$ plane for data set 3 scaled on data set 2. Map borders 5.1 by 5.1 Å. Map borders and contour interval as for Fig. 1.

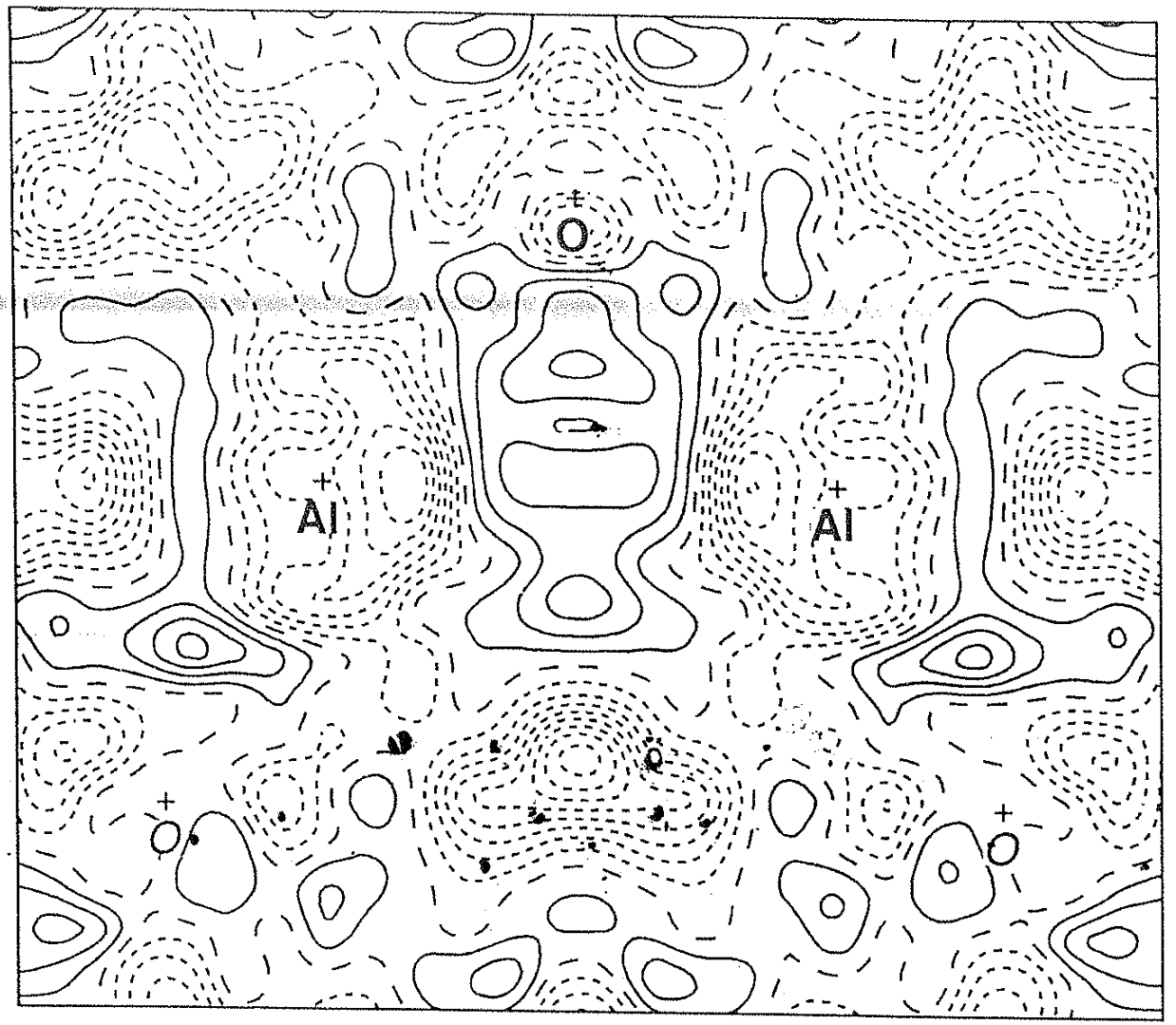

Fig. 1(a)

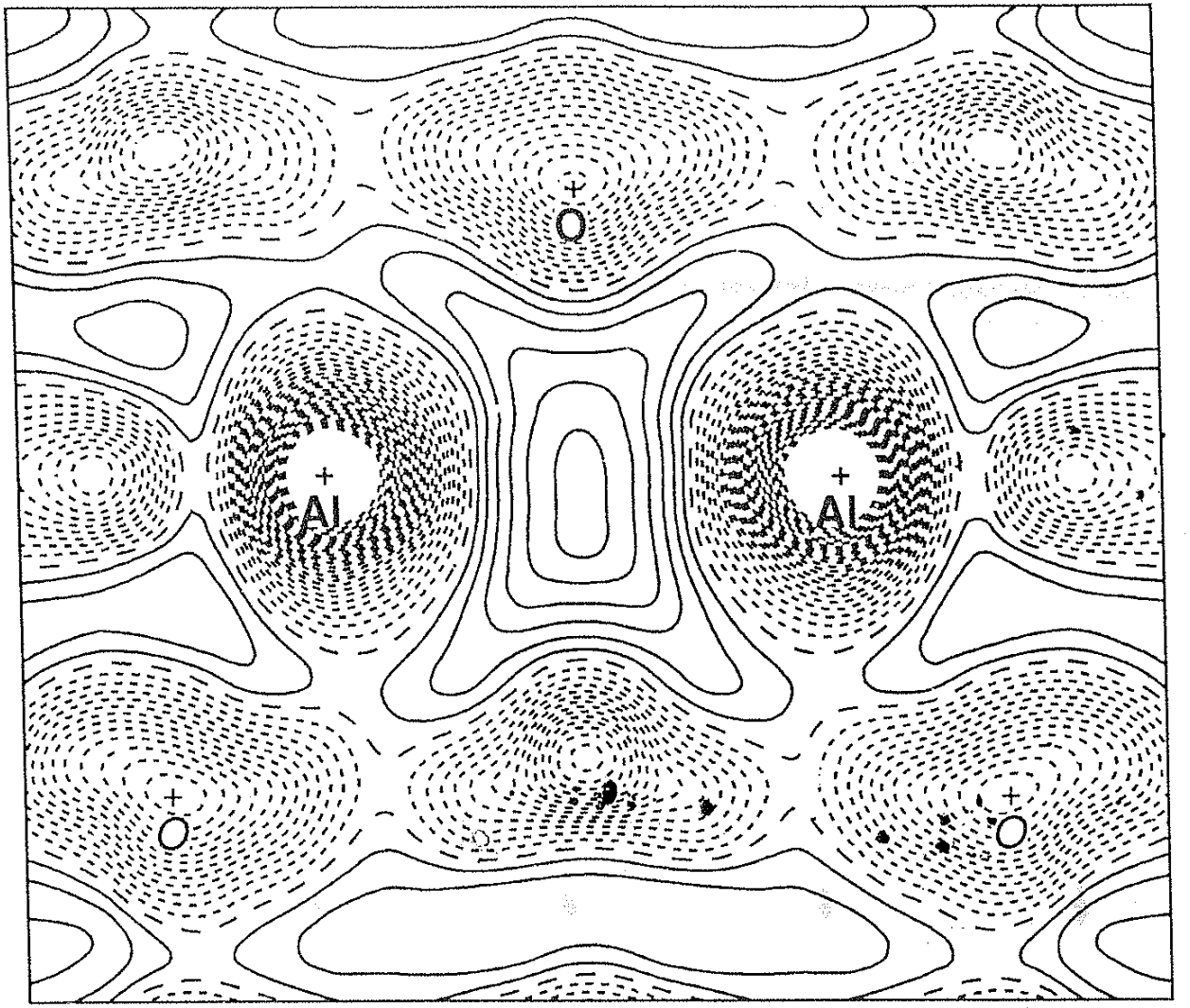

Fig. 1(b)

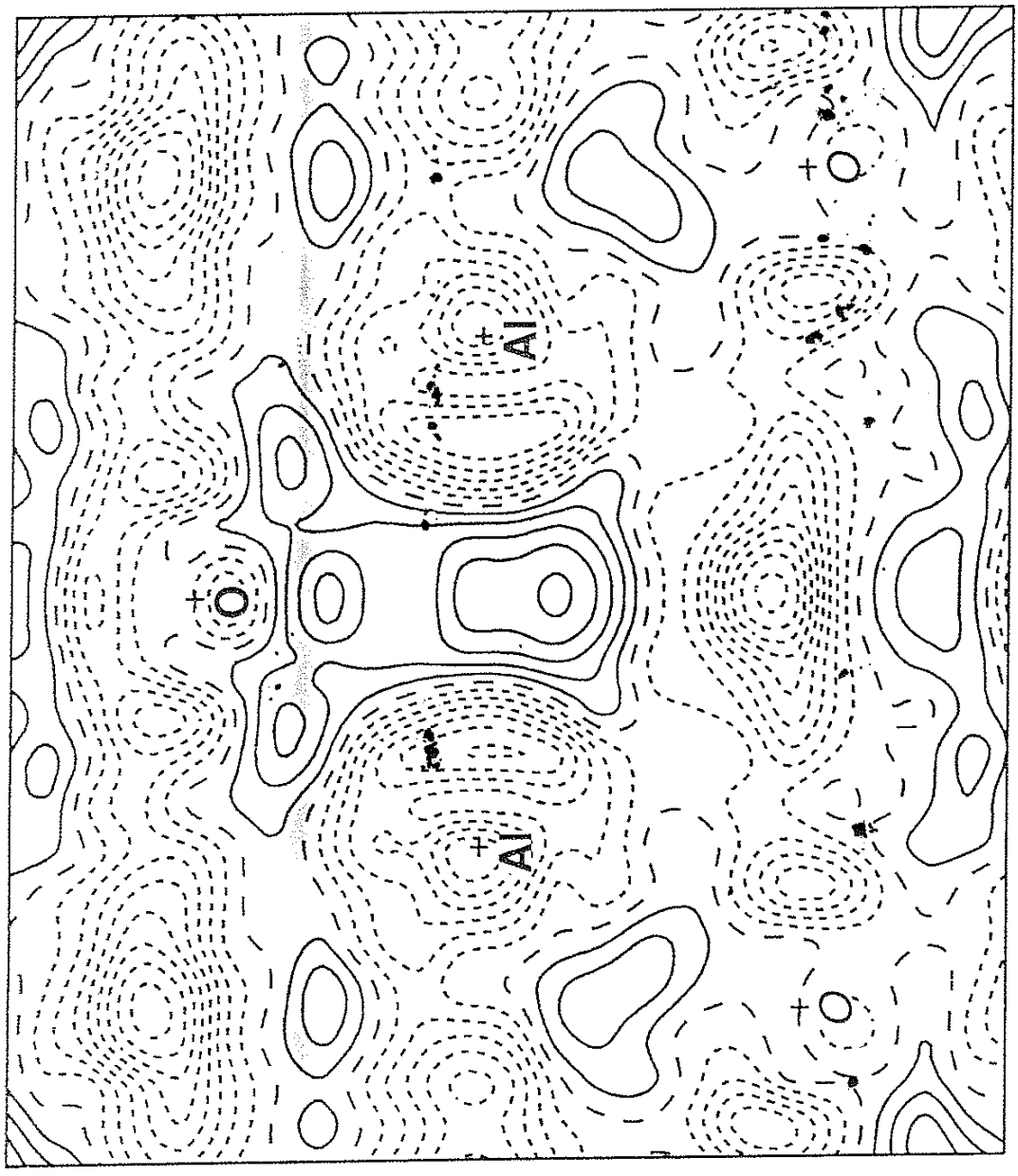

Fig. 1(c)

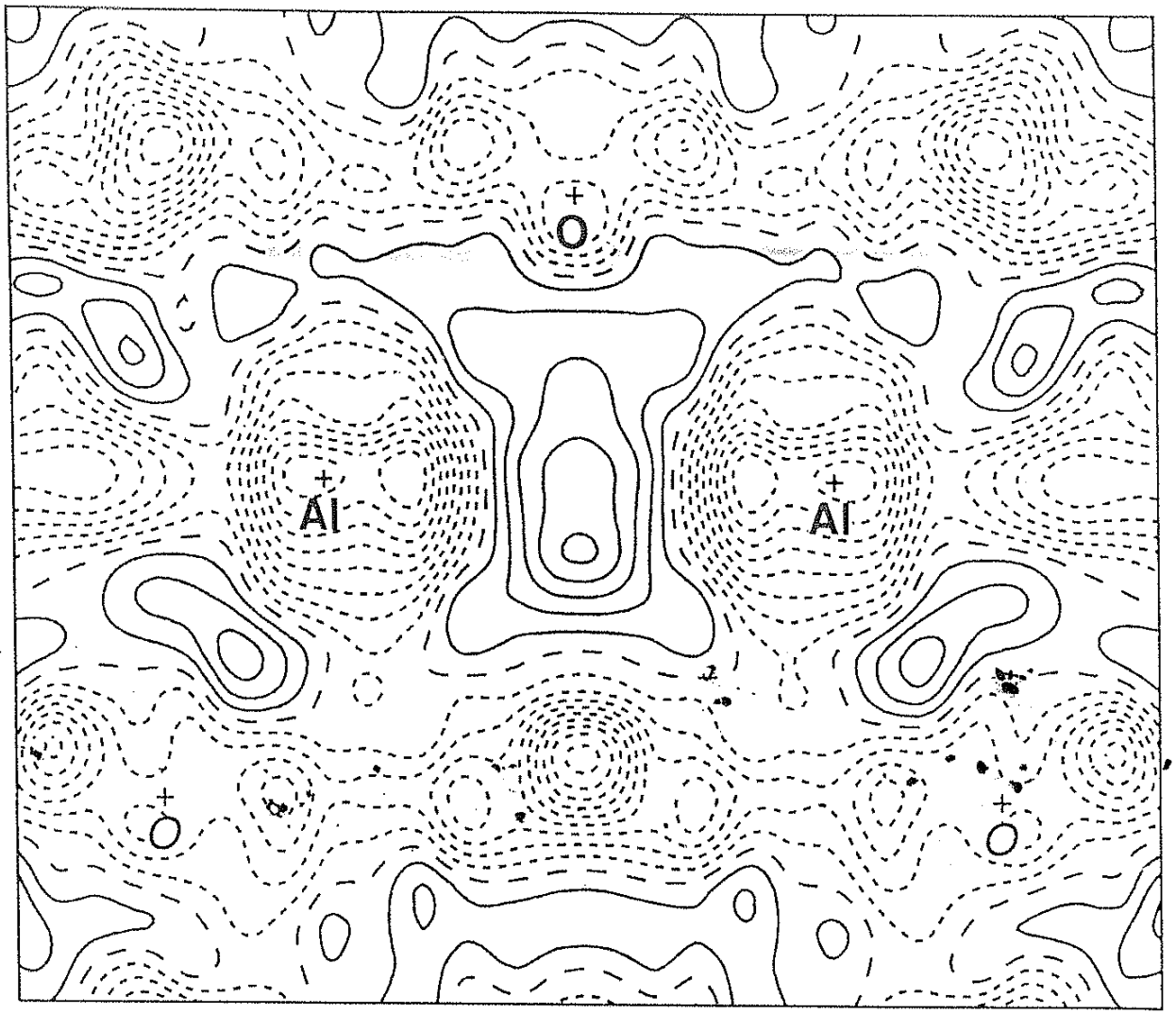

Fig. 1(d)

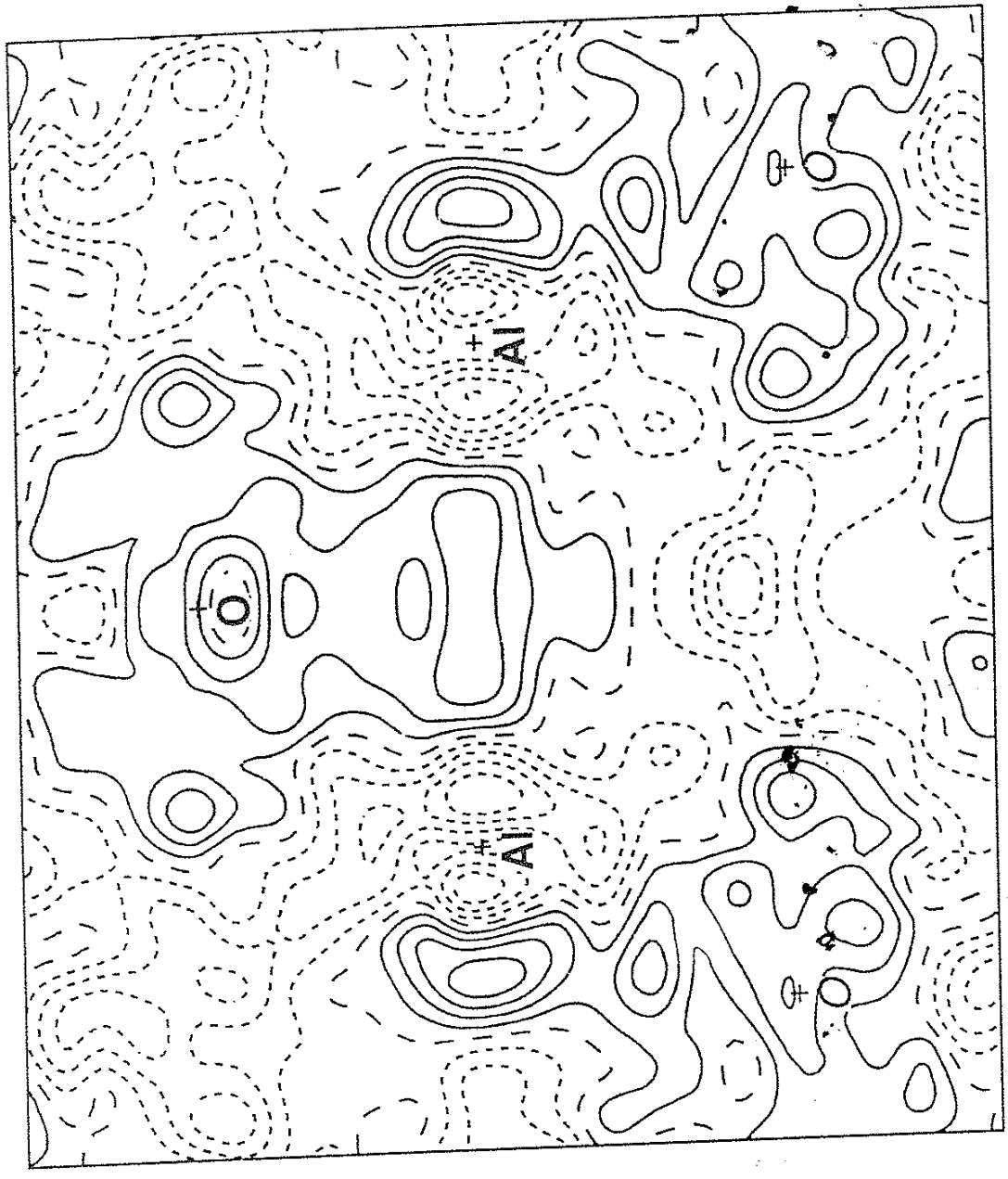

Fig. 2(a)

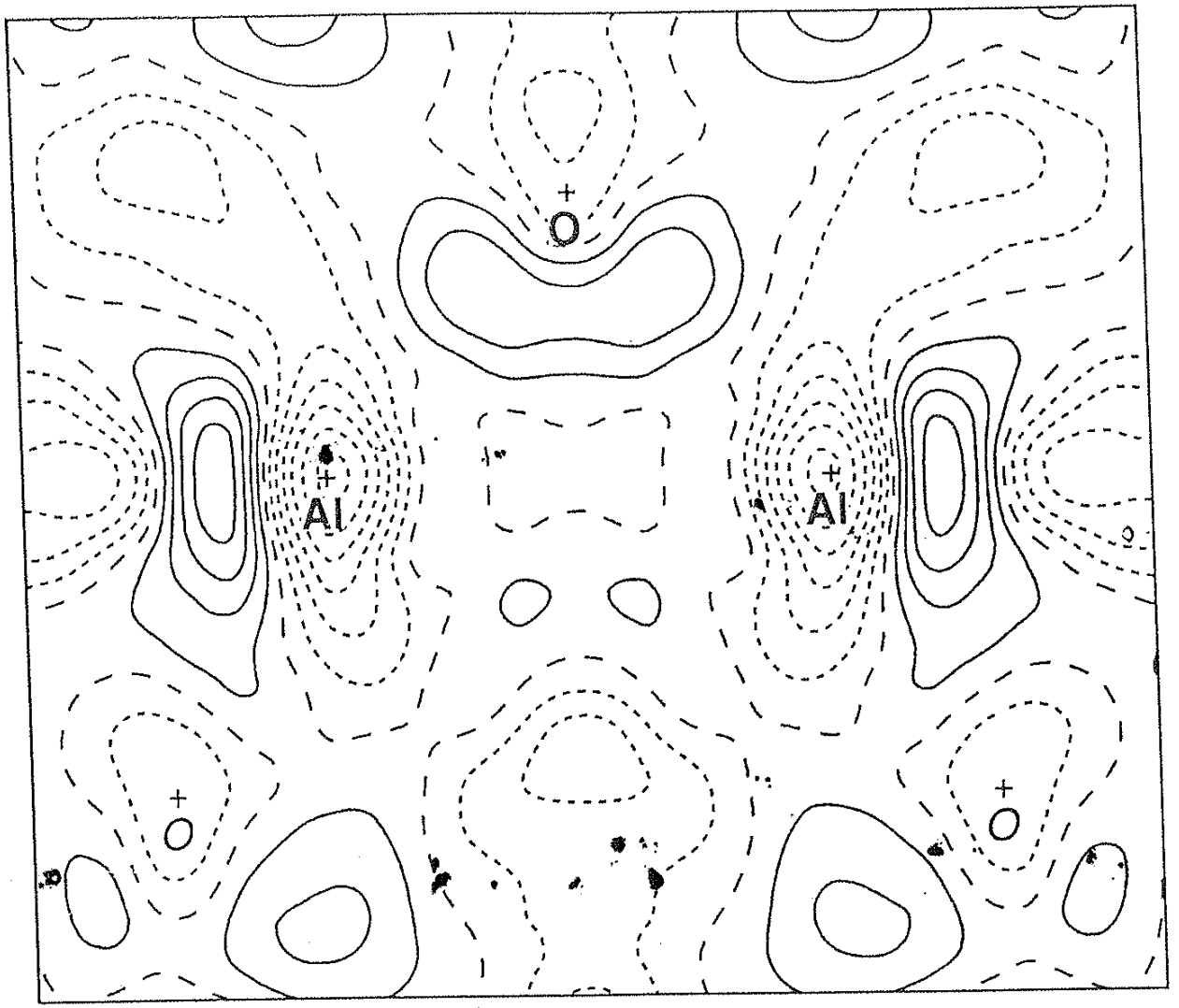

Fig. 2(b)

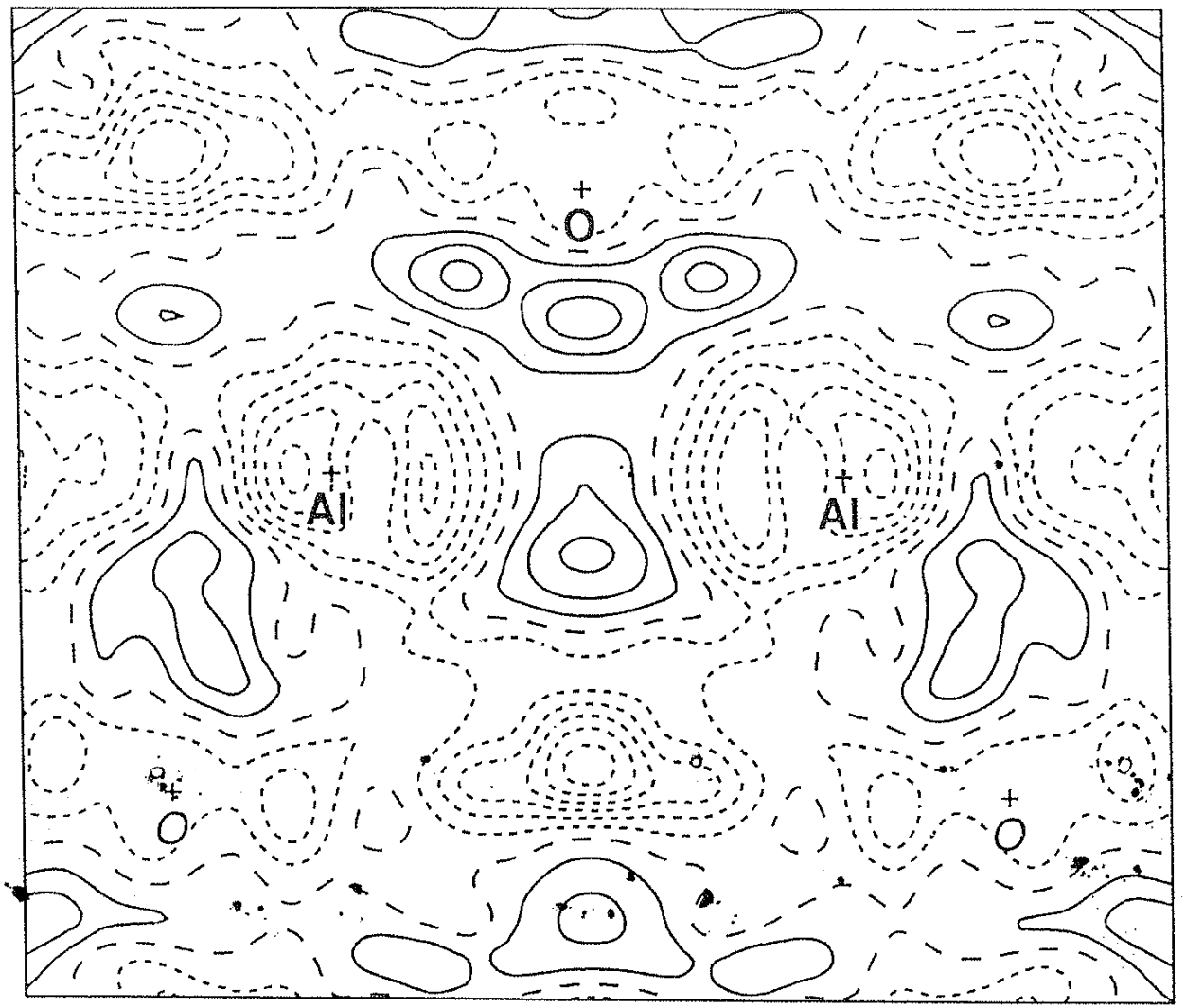

Fig. 2(c)

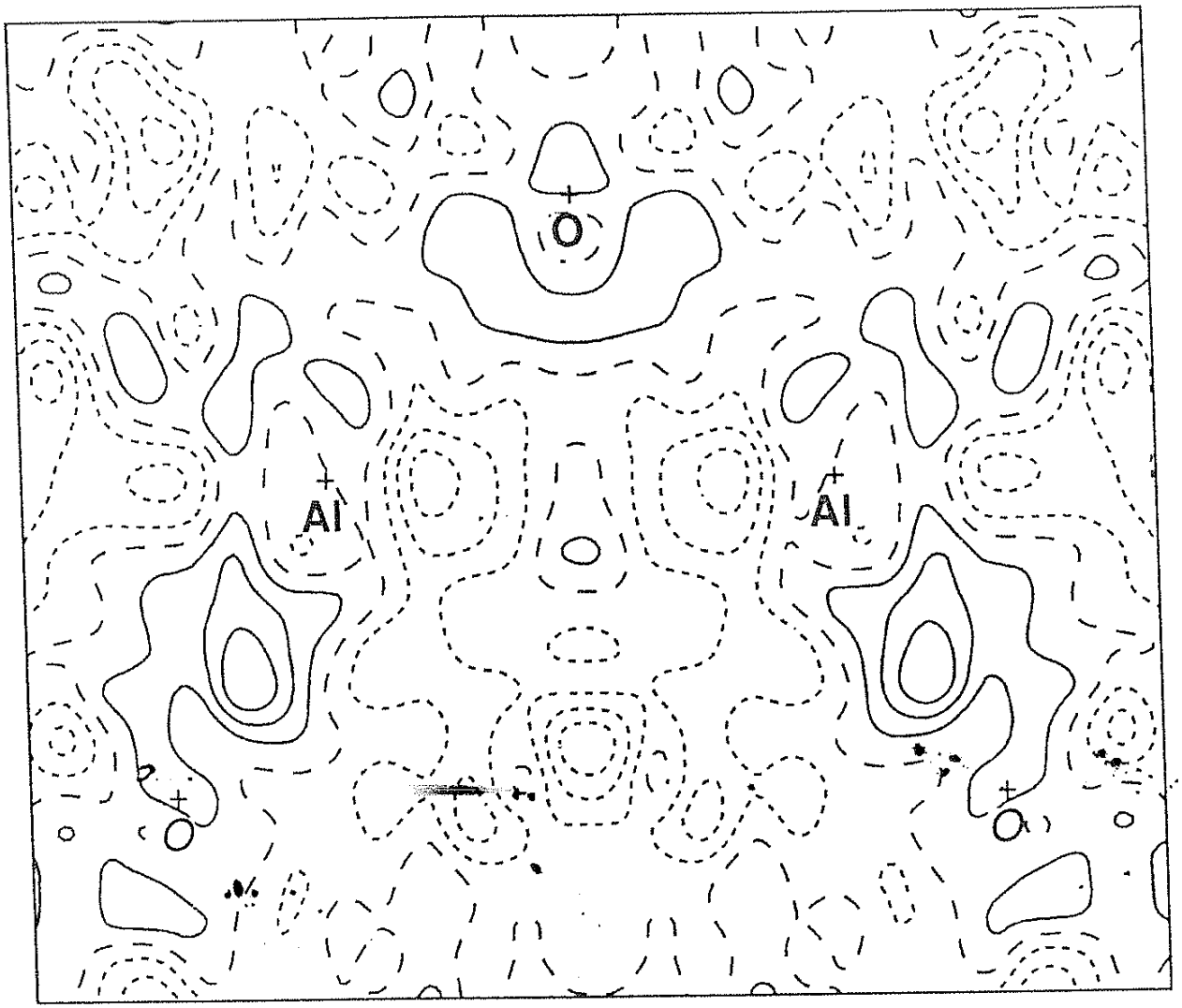

Fig. 2(d)

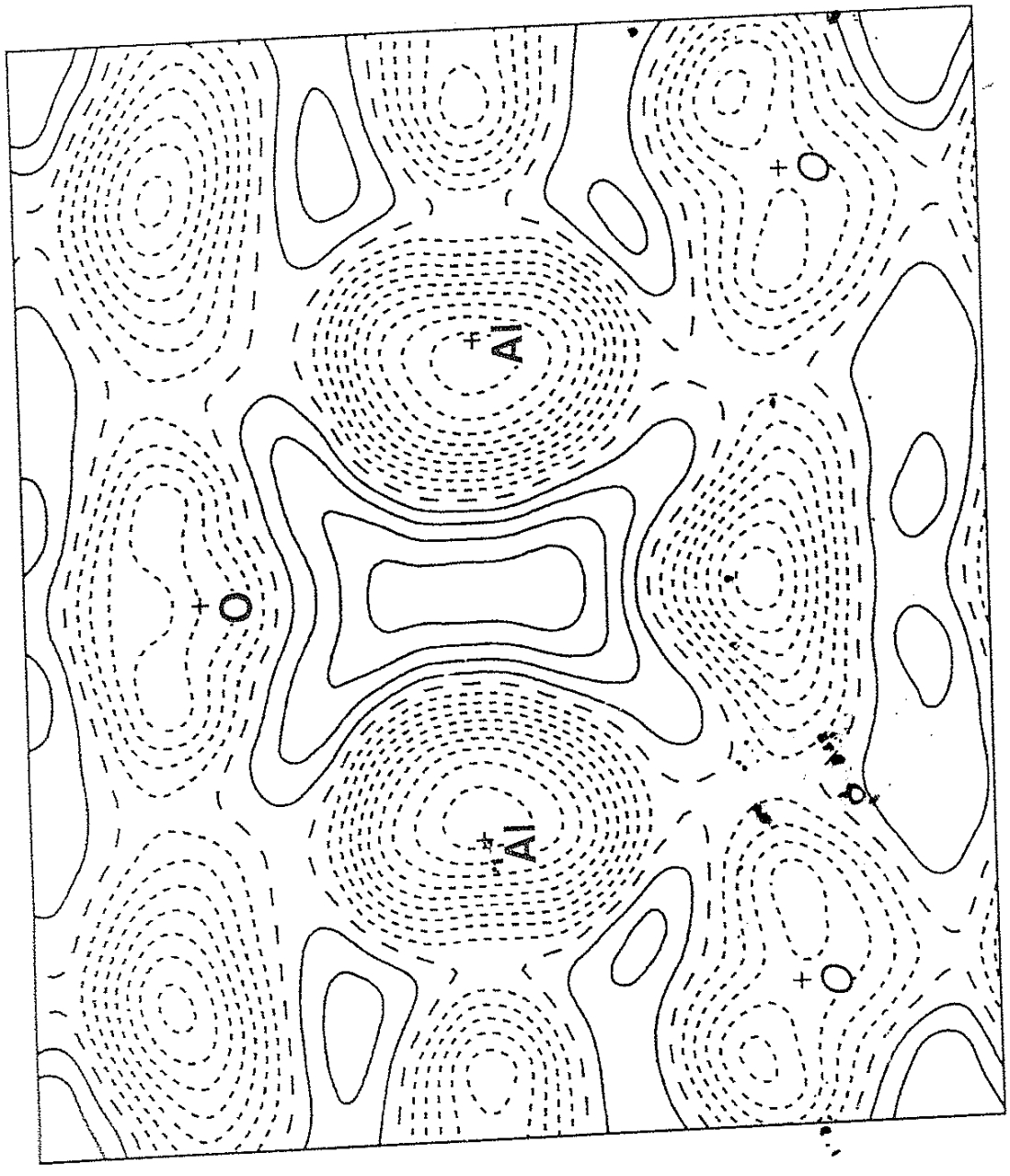

Fig. 3