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Comment on "Prediction of lattice constant in cubic perovskites"

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Abstract

In a recent work by Jiang et al. [Prediction of lattice constant in cubic perovskites, J. Phys. Chem. Solids 67 (2006) 1531–1536], the interrelationship between lattice constant, ionic radii and tolerance factor of cubic perovskites has been established and an empirical equation was obtained. However, the assumption of incorrect ionic coordination led to an incorrect mathematical expression even though the average relative errors between predicted and observed lattice constants of 132 materials were below 1%. Here, corrected coefficients for that empirical expression are obtained, which would likely be useful for investigation of general perovskite materials.

Keywords: A. Oxides; A. Inorganic compounds; A. Semiconductors; B. Epitaxial growth; B. Crystal growth

The prediction of lattice constant values for perovskite materials is of recognized importance, owing to the development of new materials designed for different applications, such as ferroelectric thin films, microwave and semiconductor technologies etc. [1–6]. Therefore, the methodology developed by Jiang et al. [1], which allows one to predict the lattice constants (a_{pred}) of cubic perovskites (ABX_3) by using the known ionic radii of the cations and anion, appears to be very useful and should likely become a key reference for materials scientists and engineers working in the field [7–10]. However, in their work, Jiang et al. used ionic radii of all ions A, B and X, for coordination numbers (CN) equal to 6, obtaining an incorrect expression for a_{pred} as a function of the ionic radii and tolerance factor. Once we truly believe on the importance of that procedure, the purpose of this work is to present the corrected coefficients for the Jiang's expression.

In perovskite structures, B cations are coordinated by six X anions, while A cations present CN = 12 (also coordinated by X anions). The X anions have CN = 2, being coordinated by two B cations, since the distance $A-O$ is about 40% larger than the $B-O$ bond distance. The correct ionic radii (r_A, r_B, r_X), taken from Shannon's work [11] and other references [12–16] are presented in Table 1. Tolerance factors $\{t = (r_A + r_X)/[\sqrt{2}(r_B + r_X)]\}$ were recalculated and new coefficients (β, δ and γ) for Jiang's expression, $a_{pred} = 2\beta(r_B + r_X) + \gamma t - \delta$, were obtained. These coefficients are summarized in Tables 1 and 2, together with two sets of Jiang's coefficients and with the average relative errors for the 132 materials used for determining Jiang's expression. The second set (Jiang[b]) was determined after using the correct β value obtained by those authors.

The difference in the empirical coefficients can be easily seen from the plots of lattice constant (a) versus $2(r_B + r_X)$, presented in Fig. 1, and $[2\beta(r_B + r_X) - a]$ versus the tolerance factor (t), Fig. 2, with the β values determined from the fits of Fig. 1. It can be seen that the correction of the ionic radii of A and X ions led to smaller $2(r_B + r_X)$ and larger t values, shifting the data in the figures and changing the fitting parameters. However, the linear trends in all cases are maintained, and the fits of the curves give $a = \alpha + 2\beta(r_B + r_X)$ in Fig. 1, and $2\beta(r_B + r_X) - a = -\gamma t + \delta$, in Fig. 2.

It is worthy noticing that an ideal cubic perovskite would have $t \approx 1$, while materials with smaller t values usually

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Table 1
Ionic radii and lattice parameters for 132 perovskites (compound 57 is meaningless)

No.	Compound	a (Å)	r_A (Å)	r_B (Å)	r_X (Å)	t	$2(r_B + r_X)$	$2\beta(r_B + r_X) - a$	a_{pred} (Å)	Dev. (%)
1	$CsIO_3$	4.674	1.88	0.95	1.35	0.993	4.60	−0.484	4.539	2.883
2	$RbUO_3$	4.323	1.72	0.76	1.35	1.029	4.22	−0.479	4.234	2.064
3	KUO_3	4.29	1.64	0.76	1.35	1.002	4.22	−0.446	4.203	2.021
4	$RbPaO_3$	4.368	1.72	0.78	1.35	1.019	4.26	−0.488	4.259	2.490
5	$KPaO_3$	4.341	1.64	0.78	1.35	0.993	4.26	−0.461	4.229	2.579
6	$KTaO_3$	3.988	1.64	0.64	1.35	1.062	3.98	−0.363	4.053	1.638
7	$BaFeO_3$	3.994	1.61	0.585	1.35	1.082	3.87	−0.469	3.975	0.476
8	$BaMoO_3$	4.040	1.61	0.65	1.35	1.047	4.00	−0.396	4.053	0.333
9	$BaNbO_3$	4.080	1.61	0.68	1.35	1.031	4.06	−0.382	4.091	0.259
10	$BaSnO_3$	4.116	1.61	0.69	1.35	1.026	4.08	−0.400	4.103	0.315
11	$BaHfO_3$	4.171	1.61	0.71	1.35	1.016	4.12	−0.418	4.128	1.027
12	$BaZrO_3$	4.193	1.61	0.72	1.35	1.011	4.14	−0.422	4.141	1.245
13	$BaIrO_3$	4.100	1.61	0.625	1.35	1.060	3.95	−0.502	4.023	1.879
14	$EuTiO_3$	3.905	1.23	0.67	1.35	0.903	4.04	−0.225	3.927	0.565
15	$NaWO_3$	3.850	1.39	0.62	1.35	0.983	3.94	−0.261	3.927	2.006
16	$SnTaO_3$	3.880	1.10	0.68	1.35	0.853	4.06	−0.182	3.889	0.227
17	$SrMnO_3$	3.806	1.44	0.53	1.35	1.049	3.76	−0.381	3.838	0.843
18	$SrVO_3$	3.890	1.44	0.58	1.35	1.022	3.86	−0.374	3.898	0.214
19	$SrFeO_3$	3.850	1.44	0.585	1.35	1.020	3.87	−0.325	3.904	1.415
20	$SrTiO_3$	3.905	1.44	0.605	1.35	1.009	3.91	−0.343	3.929	0.615
21	$SrTcO_3$	3.949	1.44	0.645	1.35	0.989	3.99	−0.315	3.979	0.757
22	$SrMoO_3$	3.975	1.44	0.65	1.35	0.986	4.00	−0.331	3.985	0.257
23	$SrNbO_3$	4.016	1.44	0.68	1.35	0.972	4.06	−0.318	4.023	0.182
24	$SrSnO_3$	4.034	1.44	0.69	1.35	0.967	4.08	−0.318	4.036	0.052
25	$SrHfO_3$	4.069	1.44	0.71	1.35	0.958	4.12	−0.316	4.062	0.175
26	$CaVO_3$	3.767	1.34	0.58	1.35	0.986	3.86	−0.251	3.857	2.381
27	$BaPbO_3$	4.265	1.61	0.775	1.35	0.985	4.25	−0.394	4.211	1.260
28	$BaTbO_3$	4.285	1.61	0.76	1.35	0.992	4.22	−0.441	4.192	2.173
29	$BaPrO_3$	4.354	1.61	0.85	1.35	0.951	4.40	−0.346	4.310	1.016
30	$BaCeO_3$	4.397	1.61	0.87	1.35	0.943	4.44	−0.353	4.336	1.376
31	$BaAmO_3$	4.357	1.61	0.85	1.35	0.951	4.40	−0.349	4.310	1.084
32	$BaNpO_3$	4.384	1.61	0.87	1.35	0.943	4.44	−0.340	4.336	1.084
33	$BaUO_3$	4.387	1.61	0.89	1.35	0.934	4.48	−0.306	4.363	0.539
34	$BaPaO_3$	4.450	1.61	0.9	1.35	0.930	4.50	−0.351	4.377	1.644
35	$BaThO_3$	4.480	1.61	0.94	1.35	0.914	4.58	−0.308	4.431	1.088
36	$SrTbO_3$	4.180	1.44	0.76	1.35	0.935	4.22	−0.336	4.127	1.263
37	$SrAmO_3$	4.230	1.44	0.85	1.35	0.897	4.40	−0.222	4.248	0.419
38	$SrPuO_3$	4.280	1.44	0.86	1.35	0.893	4.42	−0.254	4.261	0.436
39	$SrCoO_3$	3.850	1.44	0.53	1.35	1.049	3.76	−0.425	3.838	0.309
40	$BaTiO_3$	4.012	1.61	0.605	1.35	1.071	3.91	−0.450	3.999	0.328
41	$CaTiO_3$	3.840	1.34	0.605	1.35	0.973	3.91	−0.278	3.888	1.248
42	$CeAlO_3$	3.772	1.34	0.535	1.35	1.009	3.77	−0.338	3.801	0.781
43	$EuAlO_3$	3.725	1.23	0.535	1.35	0.968	3.77	−0.291	3.755	0.794
44	$EuCrO_3$	3.803	1.23	0.615	1.35	0.928	3.93	−0.223	3.856	1.383
45	$EuFeO_3$	3.836	1.23	0.645	1.35	0.914	3.99	−0.206	3.894	1.522
46	$GdAlO_3$	3.710	1.22	0.535	1.35	0.964	3.77	−0.276	3.750	1.087
47	$GdCrO_3$	3.795	1.22	0.615	1.35	0.925	3.93	−0.215	3.852	1.489

48	$GdFeO_3$	3.820	1.22	0.645	1.35	0.911	3.99	−0.186	3.890	1.842
49	$KNbO_3$	4.007	1.64	0.64	1.35	1.062	3.98	−0.382	4.053	1.156
50	$LaAlO_3$	3.778	1.36	0.535	1.35	1.017	3.77	−0.344	3.810	0.846
51	$LaCrO_3$	3.874	1.36	0.615	1.35	0.975	3.93	−0.294	3.909	0.896
52	$LaFeO_3$	3.920	1.36	0.645	1.35	0.961	3.99	−0.286	3.947	0.681
53	$LaGaO_3$	3.874	1.36	0.62	1.35	0.973	3.94	−0.285	3.915	1.058
54	$LaRhO_3$	3.940	1.36	0.665	1.35	0.951	4.03	−0.269	3.972	0.820
55	$LaTiO_3$	3.920	1.36	0.67	1.35	0.949	4.04	−0.240	3.979	1.499
56	$LaVO_3$	3.910	1.36	0.64	1.35	0.963	3.98	−0.285	3.940	0.776
57	$NaAlO_3$	3.730	1.39	0.535	1.35	1.028	3.77	−0.296	3.823	2.486
58	$NaTaO_3$	3.881	1.39	0.64	1.35	0.974	3.98	−0.256	3.952	1.841
59	$NdAlO_3$	3.752	1.27	0.535	1.35	0.983	3.77	−0.320	3.772	0.523
60	$NdCoO_3$	3.777	1.27	0.545	1.35	0.978	3.79	−0.325	3.784	0.184
61	$NdCrO_3$	3.835	1.27	0.615	1.35	0.943	3.93	−0.255	3.872	0.963
62	$NdFeO_3$	3.870	1.27	0.645	1.35	0.929	3.99	−0.236	3.910	1.046
63	$NdMnO_3$	3.800	1.27	0.645	1.35	0.929	3.99	−0.166	3.910	2.907
64	$PrAlO_3$	3.757	1.30	0.535	1.35	0.994	3.77	−0.323	3.784	0.729
65	$PrCrO_3$	3.852	1.30	0.615	1.35	0.954	3.93	−0.272	3.884	0.835
66	$PrFeO_3$	3.887	1.30	0.645	1.35	0.939	3.99	−0.253	3.923	0.915
67	$PrGaO_3$	3.863	1.30	0.62	1.35	0.951	3.94	−0.274	3.891	0.713
68	$PrMnO_3$	3.820	1.30	0.645	1.35	0.939	3.99	−0.186	3.923	2.685
69	$PrVO_3$	3.890	1.30	0.64	1.35	0.942	3.98	−0.265	3.916	0.672
70	$SmAlO_3$	3.734	1.24	0.535	1.35	0.972	3.77	−0.300	3.759	0.665
71	$SmCoO_3$	3.750	1.24	0.545	1.35	0.966	3.79	−0.298	3.771	0.567
72	$SmVO_3$	3.890	1.24	0.64	1.35	0.920	3.98	−0.265	3.892	0.049
73	$SmFeO_3$	3.845	1.24	0.645	1.35	0.918	3.99	−0.211	3.898	1.389
74	$SrZrO_3$	4.101	1.44	0.72	1.35	0.953	4.14	−0.330	4.075	0.638
75	$YAlO_3$	3.680	1.20	0.535	1.35	0.957	3.77	−0.246	3.742	1.679
76	$YCrO_3$	3.768	1.20	0.615	1.35	0.918	3.93	−0.188	3.843	1.999
77	$YFeO_3$	3.785	1.20	0.645	1.35	0.904	3.99	−0.151	3.882	2.570
78	$CsCdF_3$	4.470	1.88	0.95	1.285	1.001	4.47	−0.398	4.430	0.888
79	$CsCaF_3$	4.523	1.88	1.00	1.285	0.979	4.57	−0.360	4.496	0.586
80	$CsHgF_3$	4.570	1.88	1.02	1.285	0.971	4.61	−0.371	4.523	1.023
81	$CsSrF_3$	4.750	1.88	1.18	1.285	0.908	4.93	−0.259	4.743	0.147
82	$TlCoF_3$	4.138	1.70	0.745	1.285	1.040	4.06	−0.440	4.100	0.907
83	$TlFeF_3$	4.188	1.70	0.78	1.285	1.022	4.13	−0.426	4.144	1.046
84	$TlMnF_3$	4.260	1.70	0.83	1.285	0.998	4.23	−0.407	4.208	1.224
85	$TlCdF_3$	4.400	1.70	0.95	1.285	0.944	4.47	−0.328	4.366	0.782
86	NH_4ZnF_3	4.115	1.80	0.74	1.285	1.077	4.05	−0.426	4.134	0.459
87	NH_4CoF_3	4.129	1.80	0.745	1.285	1.075	4.06	−0.431	4.140	0.266
88	NH_4FeF_3	4.177	1.80	0.78	1.285	1.056	4.13	−0.415	4.183	0.145
89	NH_4MnF_3	4.241	1.80	0.83	1.285	1.031	4.23	−0.388	4.246	0.113
90	$RbZnF_3$	4.122	1.72	0.74	1.285	1.049	4.05	−0.433	4.102	0.481
91	$RbCoF_3$	4.141	1.72	0.745	1.285	1.047	4.06	−0.443	4.108	0.788
92	$RbVF_3$	4.170	1.72	0.79	1.285	1.024	4.15	−0.390	4.165	0.131
93	$RbFeF_3$	4.174	1.72	0.78	1.285	1.029	4.13	−0.412	4.152	0.528
94	$RbMnF_3$	4.240	1.72	0.83	1.285	1.005	4.23	−0.387	4.215	0.579
95	$RbCdF_3$	4.398	1.72	0.95	1.285	0.951	4.47	−0.326	4.373	0.573
96	$RbCaF_3$	4.452	1.72	1.00	1.285	0.930	4.57	−0.289	4.440	0.264
97	$RbHgF_3$	4.470	1.72	1.02	1.285	0.922	4.61	−0.271	4.468	0.055
98	$KCdF_3$	4.293	1.64	0.95	1.285	0.925	4.47	−0.221	4.344	1.189
99	$KMgF_3$	3.989	1.64	0.72	1.285	1.032	4.01	−0.336	4.046	1.419

Table 1 (*continued*)

No.	Compound	a (Å)	r_A (Å)	r_B (Å)	r_X (Å)	t	$2(r_B + r_X)$	$2\beta(r_B + r_X) - a$	a_{pred} (Å)	Dev. (%)
100	$KNiF_3$	4.013	1.64	0.69	1.285	1.047	3.95	−0.415	4.009	0.106
101	$KZnF_3$	4.056	1.64	0.74	1.285	1.021	4.05	−0.367	4.070	0.356
102	$KCoF_3$	4.071	1.64	0.745	1.285	1.019	4.06	−0.373	4.077	0.140
103	KVF_3	4.100	1.64	0.79	1.285	0.997	4.15	−0.320	4.134	0.819
104	$KFeF_3$	4.121	1.64	0.78	1.285	1.002	4.13	−0.359	4.121	0.003
105	$KMnF_3$	4.189	1.64	0.83	1.285	0.978	4.23	−0.336	4.185	0.094
106	$AgMgF_3$	3.918	1.48	0.72	1.285	0.975	4.01	−0.265	3.982	1.621
107	$AgNiF_3$	3.936	1.48	0.69	1.285	0.990	3.95	−0.338	3.944	0.195
108	$AgZnF_3$	3.972	1.48	0.74	1.285	0.966	4.05	−0.283	4.007	0.881
109	$AgCoF_3$	3.983	1.48	0.745	1.285	0.963	4.06	−0.285	4.013	0.764
110	$AgMnF_3$	4.030	1.48	0.83	1.285	0.924	4.23	−0.177	4.124	2.340
111	$NaVF_3$	3.940	1.39	0.79	1.285	0.912	4.15	−0.160	4.037	2.458
112	$RbPdF_3$	4.298	1.72	0.86	1.285	0.991	4.29	−0.390	4.254	1.021
113	NH_4MgF_3	4.060	1.80	0.72	1.285	1.088	4.01	−0.407	4.110	1.223
114	$TlPdF_3$	4.301	1.70	0.86	1.285	0.984	4.29	−0.393	4.247	1.264
115	$LiBaF_3$	3.992	1.61	0.76	1.285	1.001	4.09	−0.267	4.084	2.299
116	$RbYbF_3$	4.530	1.72	1.02	1.285	0.922	4.61	−0.331	4.468	1.379
117	$CsEuF_3$	4.780	1.88	1.17	1.285	0.912	4.91	−0.308	4.729	1.064
118	$CsPbF_3$	4.800	1.88	1.19	1.285	0.904	4.95	−0.291	4.757	0.891
119	$CsYbF_3$	4.610	1.88	1.02	1.285	0.971	4.61	−0.411	4.523	1.882
120	$RbPbF_3$	4.790	1.72	1.19	1.285	0.859	4.95	−0.281	4.705	1.768
121	$CsCaCl_3$	5.396	1.88	1.00	1.79	0.930	5.58	−0.313	5.360	0.658
122	$CsCdCl_3$	5.210	1.88	0.95	1.79	0.947	5.48	−0.218	5.289	1.510
123	$CsPbCl_3$	5.605	1.88	1.19	1.79	0.871	5.96	−0.176	5.639	0.612
124	$CsHgCl_3$	5.410	1.88	1.02	1.79	0.924	5.62	−0.291	5.389	0.381
125	$TlMnCl_3$	5.020	1.70	0.83	1.79	0.942	5.24	−0.247	5.064	0.880
126	$CsEuCl_3$	5.627	1.88	1.17	1.79	0.877	5.92	−0.235	5.610	0.311
127	$CsTmCl_3$	5.476	1.88	1.03	1.79	0.920	5.64	−0.339	5.404	1.317
128	$CsYbCl_3$	5.437	1.88	1.02	1.79	0.924	5.62	−0.318	5.389	0.875
129	$CsHgBr_3$	5.770	1.88	1.02	1.95	0.912	5.94	−0.359	5.668	1.774
130	$CsPbBr_3$	5.874	1.88	1.19	1.95	0.862	6.28	−0.154	5.921	0.805
131	$CsSnBr_3$	5.795	1.88	0.95	1.95	0.934	5.80	−0.512	5.565	3.967
132	$CsSnI_3$	6.219	1.88	0.95	2.16	0.919	6.22	−0.553	5.930	4.642
								Average deviation (%)		1.07

Ionic radii for Cl, Br, I, Ag, Sn, and lanthanides from Refs. [12–16].

Table 2
Empirical coefficients for determining the lattice constants of cubic perovskites, with the expression $a_{pred} = 2\beta(r_B + r_X) + \gamma t - \delta$

	β	γ	δ	% error
Jiang[a]	0.9418	1.4898	1.2062	0.63
Jiang[b]	0.9148	1.4314	1.0368	0.63
This work	0.9109	1.1359	0.7785	1.07

Jiang[a] are the coefficients given in Ref. [1] with incorrect β value; Jiang[b] are the coefficients with correct β value for the same work.

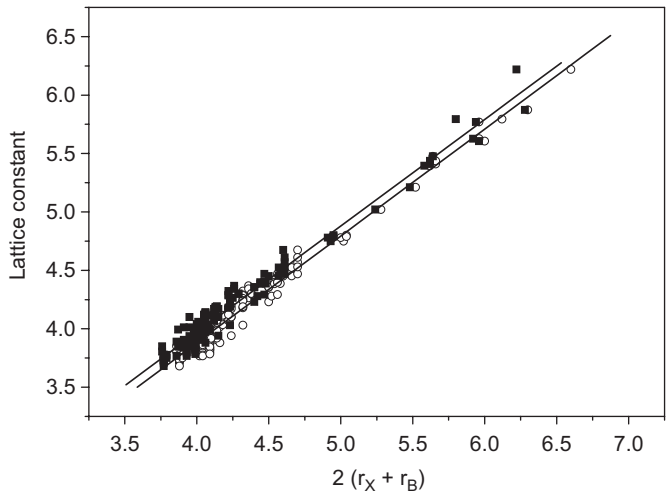

Fig. 1. Linear fits used for determining the β parameter. Here, $a = \alpha + 2\beta(r_B + r_X)$. Open circles for data of Ref. [1]; full squares are our corrected data. Both axes in Angstroms.

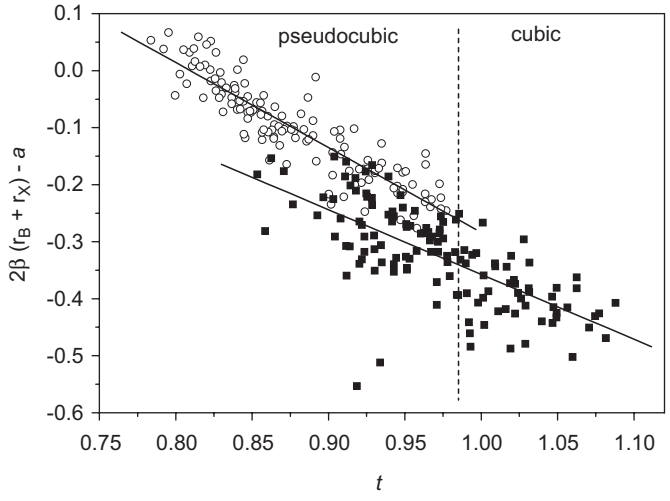

Fig. 2. Linear fits of $2\beta(r_B + r_X) - a = -\gamma t + \delta$, for obtaining the parameters γ and δ. Same symbols as in Fig. 1. The dashed line indicates the critical line for cubic structures. Vertical axis in Angstroms.

belong to lower symmetry structures, with tilted BX_6 octahedra [17]. The critical t value for stabilizing cubic structures is about 0.985 [17]. This value is higher than those obtained in Ref. [1] for all the 132 materials investigated. Take for instance $SrTiO_3$: according to Ref. [1], this material would present $t = 0.908$, indicating that it would belong to a distorted/tilted non-cubic structure; after the correction proposed here, t becomes 1.009, in agreement with its experimentally observed untilted cubic structure (at room temperature) [18]. Another remark concerns the increase in the average deviation between predicted and experimental lattice parameters. As it can be seen in Fig. 2, the dispersion of data increased after correction of the CN's. This could be due to a lower accuracy of ionic radii used for CN = 12 (worse statistics than for CN = 6), although we should remember that most structures are indeed pseudocubic, with tilted BX_6 octahedra, which change both, the approximated a value (i.e., the cubic ratio of the unit cell volume) as well as the "average" ionic radii used in the calculations.

In conclusion, we believe that the empirical expression for determining the lattice parameters of cubic perovskites developed in Ref. [1], with the corrections presented here, could be very useful in future researches in this field.

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