TABLE II. General Cauchy relations for first-, second-, and third-order elastic constants. Also listed are coefficients used in the general expressions for the elastic constants.

Types *ijklmn*	Elastic constants with Cauchy relations $C_{ij}\ldots$	$X_{ij}\ldots$	$Y_{ijkl}\ldots$	Z_{ijklmn}
	First order			
II	$C_1,\ C_2,\ C_3$	1		
JK	$C_4,\ C_5,\ C_6$	0		
	Second order			
IIII	$C_{11},\ C_{22},\ C_{33}$	3	$6g_I^2$	
IIJJ	$C_{12}=C_{66},\ C_{13}=C_{55},\ C_{23}=C_{44}$	1	$g_I^2+g_J^2$	
JJJK	$C_{15},\ C_{16},\ C_{24},\ C_{26},\ C_{34},\ C_{35}$	0	$3g_Jg_K$	
IJK	$C_{14}=C_{56},\ C_{25}=C_{46},\ C_{36}=C_{45}$	0	g_Jg_K	
	Third order			
IIIII	$C_{111},\ C_{222},\ C_{333}$	15	$45g_I^2$	$15g_I^4$
IIIJJ	$C_{112}=C_{166},\ C_{113}=C_{155},\ C_{122}=C_{266}$ $C_{133}=C_{355},\ C_{223}=C_{244},\ C_{233}=C_{344}$	3	$6g_I^2+3g_J^2$	$g_I^4+6g_I^2g_J^2$
IIJJKK	$C_{123}=C_{144}=C_{255}=C_{366}=C_{456}$	1	$g_I^2+g_J^2+g_K^2$	$g_I^2g_J^2+g_J^2g_K^2+g_K^2g_I^2$
JJJJJK	$C_{115},\ C_{116},\ C_{224},\ C_{226},\ C_{334},\ C_{335}$	0	$15g_Jg_K$	$10g_J^3g_K$
JJJKKK	$C_{126}=C_{666},\ C_{135}=C_{555},\ C_{234}=C_{444}$	0	$9g_Jg_K$	$3g_Jg_K(g_J^2+g_K^2)$
IIIJK	$C_{114}=C_{156},\ C_{225}=C_{246},\ C_{336}=C_{345}$	0	$3g_Jg_K$	$6g_I^2g_Jg_K$
IIJJJK	$C_{125}=C_{146}=C_{566},\ C_{124}=C_{256}=C_{466}$ $C_{134}=C_{356}=C_{455},\ C_{136}=C_{145}=C_{556}$ $C_{235}=C_{346}=C_{445},\ C_{236}=C_{245}=C_{446}$	0	$3g_Jg_K$	$g_Jg_K(3g_I^2+g_J^2)$

elastic constants. For convenience, the $X_{ij}\ldots$, $Y_{ijkl}\ldots$, and Z_{ijklmn} coefficients, which are used in Eqs. (17)–(19) to determine $C_{ij}^{es}\ldots$, have also been listed.

Calculations have been completed for seven cubic structures, namely simple cubic, fcc, bcc, NaCl type, CsCl type, diamond, and zinc blende. The first-, second-, and third-order elastic constants with Cauchy relations for these structures are

$$C_1;\quad C_{11},\quad C_{12}=C_{44};$$

and

$$C_{111},\quad C_{112}=C_{155},\quad C_{123}=C_{144}=C_{456}.$$

The electrostatic contributions to these constants are listed in Table III in units of Z^2e^2/a^4, where a is the lattice parameter.

Four hexagonal structures, namely simple hexagonal, hcp, WC type, and wurtzite, have also been considered. For these structures, the elastic constants with Cauchy relations are

$$C_1,\ C_3;\quad C_{11},\quad C_{33},\quad C_{12}=C_{66}=\tfrac{1}{3}C_{11},\quad C_{13}=C_{44};$$

and

$$C_{111},\quad C_{222},\quad C_{112}=C_{166}=\tfrac{1}{5}(-2C_{111}+3C_{222}),$$

$$C_{122}=C_{266}=\tfrac{1}{5}(3C_{111}-2C_{222}),$$

$$C_{333},\quad C_{113}=C_{155},$$

TABLE III. Electrostatic Brugger elastic constants for cubic structures. Entries are in units of Z^2e^2/a^4, where a is the lattice constant.

	simple cubic	fcc	bcc	NaCl type	CsCl type	diamond	zinc blende
U	−1.418 648 740	−9.169 724 148	−3.639 233 450	−13.980 516 757	−2.035 361 509	−21.547 192 177	−15.131 704 416
C_1	0.472 882 913	3.056 574 716	1.213 077 817	4.660 172 252	0.678 453 836	7.182 397 392	5.043 901 472
C_{11}	−0.143 189 083	−6.849 873 626	−2.697 885 714	−25.108 469 175	2.125 129 382	−23.345 777 443	−4.053 717 061
C_{12}	−0.637 729 828	−1.159 925 261	−0.470 673 868	5.563 976 209	−2.080 245 446	0.899 292 633	−5.538 993 678
C_{111}	−1.747 954 699	34.065 579 503	9.235 126 065	164.229 593 204	−16.226 944 863	119.055 300 863	17.207 017 149
C_{112}	1.231 950 057	0.091 894 314	2.127 151 252	−19.343 623 664	2.800 648 978	−1.163 206 824	1.530 784 079
C_{123}	0.724 749 027	5.615 837 678	−1.900 933 165	10.867 366 283	4.799 929 272	−2.170 049 518	24.633 400 230

TABLE IV. Electrostatic Brugger elastic constants for hexagonal structures with ideal structure parameters. Entries are in units of Z^2e^2/a^4, where a is the lattice constant.

	simple hexagonal $(c/a=1)$	hcp $(c/a=\sqrt{\frac{8}{3}})$	WC type $(c/a=\sqrt{\frac{8}{3}})$	wurtzite $(c/a=\sqrt{\frac{8}{3}},\ u=\frac{3}{8})$
U	−1.729 575 102	−2.292 340 210	−0.873 690 983	−3.790 469 934
C_1	0.533 603 351	0.764 635 593	−0.577 163 952	1.237 266 468
C_3	0.662 368 399	0.763 069 024	2.028 018 888	1.315 936 998
C_{11}	−0.605 973 676	−1.288 353 922	2.966 252 428	−2.637 875 499
C_{33}	−0.401 414 892	−1.137 003 974	−1.637 033 899	−3.558 546 850
C_{12}	−0.201 991 225	−0.429 451 308	0.988 750 809	−0.879 291 833
C_{13}	−0.792 845 153	−0.576 101 549	−2.223 511 382	−0.194 632 072
C_{111}	2.324 128 642	5.026 701 204	−15.767 553 741	12.580 565 280
C_{222}	−0.532 222 756	2.217 541 686	−19.362 925 160	2.779 206 544
C_{333}	−0.708 777 482	5.511 268 055	2.608 789 547	26.442 451 932
C_{112}	−1.248 985 111	−0.680 155 470	−5.310 733 599	−3.364 702 185
C_{122}	1.607 366 288	2.129 004 048	−1.715 362 181	6.436 656 550
C_{113}	1.954 724 848	2.095 223 879	6.247 025 199	3.973 514 399
C_{123}	0.651 574 949	0.698 407 960	2.082 341 733	1.324 504 800
C_{133}	1.357 925 970	0.086 875 908	2.788 189 975	−4.324 858 840

$$C_{123}=C_{144}=C_{366}=C_{456}=\tfrac{1}{3}C_{113},\quad C_{133}=C_{344}\ .$$

Electrostatic contributions to these elastic constants for ideal structure parameters are listed in Table IV in units of Z^2e^2/a^4. For all the hexagonal structures, our choice of Cartesian axes (in Miller–Bravais indices) has been 1 axis = $[10\bar{1}0]$; 2 axis = $[\bar{1}2\bar{1}0]$; and 3 axis = [0001]. It should be mentioned that, for the hcp structure, Cousins[5] has chosen basal axes rotated 90° with respect to ours. Thus, his C_{111} corresponds to our C_{222}, etc. However, our choice of axes is consistent with the only two sets of measured third-order elastic constants for hcp metals.[14,15] Also the different choice of axes eliminates the discrepancy, noted by Naimon *et al.*,[16] in certain Fuchs's constants calculated by Cousins.[4]

The results presented in Tables III and IV represent a higher degree of accuracy than those of earlier calculations. However, our results are essentially in agreement with those reported earlier (fcc,[1–3,9] bcc,[1–3,6,9] NaCl and CsCl,[7] zinc blende,[8] and hcp[5]). Also, all results were checked independently by doing a Fuchs-type calculation for each structure [Eq. (11) with $\lambda=(\Omega_0')^{1/3}$]. Other useful checks are the relations

$$C^{es}_{ii}=-U_{es},\quad C^{es}_{iijj}=3U_{es},\quad C^{es}_{iijjkk}=-15U_{es}\ ,$$

where, as usual, repeated indices are to be summed. These can be easily derived, for example, by relating Fuchs and Brugger constants. All calculations were performed on IBM 360 and Xerox Sigma 5 computers. Convergence of all sums was such that the maximum error in the tabulated constants was $\pm 1\times10^{-12}$. The subroutine for the complementary error function, necessary to generate the $\Phi_{-1/2}$ functions, was from an IBM routine with a relative error of less than 4×10^{-16}.

IV. GENERAL EXPRESSIONS FOR INTERNAL-STRAIN DERIVATIVES

In order to obtain the internal-strain contribution to the elastic constants, it is sufficient to know the energy density of the homogeneously deformed lattice as a function of both external and internal strains (see Appendix A). However, since the internal strains are determined from the total energy density, the electrostatic internal-strain contribution to the elastic constants cannot be obtained directly. It is still possible, though, to determine electrostatic internal-strain derivatives of the form

$$U^{(\nu p)(\mu q)\cdots}_{ijkl\cdots}=\left(\frac{\partial^n U'_{es}}{\partial\bar{w}_p(\nu)\partial\bar{w}_q(\mu)\cdots\partial\eta_{ij}\partial\eta_{kl}\cdots}\right)_{\vec{\eta}=0,\ \vec{\bar{w}}=0} \tag{26}$$

where $\vec{\bar{w}}(\nu)$ is the internal strain associated with the νth ion of the unit ccll ($\nu=0,\ 1,\cdots,s-1$). These derivatives would be combined with those arising from other terms of the energy density, thus resulting in the total internal-strain contribution to the elastic constants.

Using the method of homogeneous deformation, derivatives of $U'_{es}(\vec{\eta},\ \vec{\bar{w}}(\nu))$ can be easily performed (see Appendix B). Introducing the dimensionless parameter $\vec{t}=[\vec{\tau}(\nu)-\vec{\tau}(\mu)]/\Omega_0^{1/3}$, as well as $\vec{r}=\vec{R}(^{l0}_{\nu\mu})/\Omega_0^{1/3}$ and $\vec{g}=\Omega_0^{1/3}\vec{G}(h)/2\pi$, the expressions for the electrostatic internal-strain derivatives through third-order are