Pramāṇa – J. Phys., Vol. 34, No. 3, March 1990, pp. 201–215. © Printed in India.

Convexity of internal energy of cubic crystal deformed to orthorhombic structure

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MS received 31 July 1989; revised 3 November 1989

Abstract. A generalized set of strain variables q_r^N, has been defined to develop the expression for a generalized set of second order and third-order elastic moduli C_{rs}^N and C_{rst}^N for a cubic crystal deformed to orthorhombic structure. The Hessain $C_{rs}^N \delta q_r \delta q_s$ and $C_{rst}^N \delta q_r \delta q_s \delta q_t$ ($r = 1$, $2 \ldots\ldots 6$; summation convention) are calculated in the new variables and compared with G-strength and S-strength, for both positive and negative loading environment.

The convexity of the internal energy relative to various choice of strain measure is examined considering up to third degree terms in the internal energy expression. The computational results for *bcc* iron is presented according to the new moduli. The stable ranges thus obtained for iron under hydrostatic compressive and tensile stresses is found to generate the classical stable range, green-stable range and stretch-stable range as the specific cases. However, *bcc* iron does not seem to follow any conventional stable ranges under hydrostatic compression, where the present generalized stable range is found satisfactory.

Keywords. Material strength; elastic constants;

PACS Nos 81·40; 62·20; 03·40

1. Introduction

Studies on ideal crystal strength was initiated in 1940 by Born, which has been extensively studied by Macmillan and Kelly (1972a, b), Milstein (1971, 1973), Thakur (1982a, b, 1985) and Hill (1975) because vast information concerning mechanical behaviour and other elastic constant dependent properties of deformed solids can be gathered from these studies.

The specification of the state of homogeneous strain in a crystal involves any six variables that define the geometry of the primitive cell. Various researchers, in practice, have adopted different sets of generalized co-ordinates q_r ($r = 1, 2, \ldots, 6$), as a measure of pure homogeneous strain for the computation of ideal strength of crystal under load. It will be very interesting to see whether there exists any set of such strain variable which can generate crystal strength (under load) somewhat different (smaller or greater) from the strength obtainable from the other conventional set of variables. Hill (1975) pointed out that a suitable measure of symmetric tensor having smooth monotone scale function $f(\lambda)$ satisfying the condition $f(1) = 0$ and $f'(1) = 1$.

In this paper we have adopted a new generalized set of strain variables, q_r^N, to get the expressions for second-order elastic constant (SOEC), C_{rs}^N, and third-order elastic constants (TOEC), C_{rst}^N, for cubic crystal deformed to orthorhombic structure. The new generalized set of strain variables, q_r^N, adopted in this paper represent the generalized form of other conventional sets of strain variables namely (i) the Green's variables used by Born school (Born 1940; Born and Furth 1940; Born and Misra 1940; Misra 1940; Furth 1941), and (ii) the stretch variables used by Macmillan and Kelly (1972a, b, 1973). The rotational symmetry of the new elastic moduli is also examined.

We further compare the strength of loaded crystal determined from new moduli with those due to the conventional ones (i.e., Green and stretch moduli). The role of third order elastic moduli in the determination of stability of loaded crystals is also investigated considering upto the third degree terms in the expansion of energy in Taylor series.

Finally the computational results for a *bcc* iron subjected to hydrostatic compressive and tensile stresses are presented according to the new set of elastic moduli, which are further compared with the results obtained from the Green-moduli and the stretch moduli.

2. Theoretical approach

In the present paper we define a new set of generalized geometric variables according to Hill's (1975) criteria under the summation convention

$$q_{ij}^N = \frac{1}{1+k}\left[\tfrac{1}{2}(\lambda p_i \lambda p_j - \delta_{ij}) + k(\lambda_{ij} - \delta_{ij})\right], \tag{1}$$

where δ_{ij} is Kroneker delta, k can assume any suitable value positive or negative, and λ_{ij} are the elements of stretch tensor, a choice of Macmillan and Kelly (1972a, b) for the generalized geometric variables defined by

$$x_i = \sum \lambda_{ij} X_j \quad (i, j = 1, 2, 3) \tag{2}$$

where X_i and x_i are, respectively, the reference and current rectangular co-ordinates of any lattice vector.

The co-ordinates corresponding to the new set of strain variables (1) may explicitly be expressed by

$$q_1^N = \frac{1}{1+k}\left[\tfrac{1}{2}(\lambda_1^2 + \lambda_5^2 + \lambda_6^2 - 1) + k(\lambda_1 - 1)\right], \tag{3}$$

$$q_4^N = \frac{1}{1+k}\left[(\lambda_2 + \lambda_3)\lambda_4 + \lambda_5\lambda_6 + 2k\lambda_4\right],$$

where the tensor notation (ij) in (1) are converted into matrix notation (r) according to the following scheme

$$\begin{array}{lll} (11)\rightarrow 1, & (22)\rightarrow 2, & (33)\rightarrow 3, \\ (23)\rightarrow 4, & (31)\rightarrow 5, & (12)\rightarrow 6. \end{array} \tag{4}$$

For $k=0$, eq. (3) reduces to

$$\begin{aligned} 2q_1^G &= \lambda_1^2 + \lambda_5^2 + \lambda_6^2 - 1, \\ q_4^G &= (\lambda_2 + \lambda_3)\lambda_4 + \lambda_5\lambda_6, \end{aligned} \tag{5}$$

which represents the coordinates, q_r^G, corresponding to the Green's strain tensor adopted by Born School (Born 1940; Born and Furth 1940; Born and Misra 1940; Misra 1940). Again if we put $k=\infty$, (3) reduces to

$$\begin{aligned} q_1^S &= \lambda_1 - 1 \\ q_4^S &= 2\lambda_4 \end{aligned} \tag{6}$$

which represents the co-ordinates corresponding to the stretch variables used by Macmillan and Kelly (1972a, b). Thus the present form of the new generalized set of strain variables, q_r^N, is capable of reproducing G-variables, q_r^G, s-variables, q_r^S in special cases. Moreover, (3) can lead to any desired set of strain variables depending upon the choice of the parameter k.

The internal energy E per unit reference cell may be expressed as a function of the geometric variables q_r^N $(r = 1, 2, \ldots)$

$$E = E(q_1, q_2, \ldots, q_6)$$

and

$$r^2 = \tfrac{1}{4}(l_1^2 a_1^2 + l_2^2 a_2^2 + l_3^2 a_3^2) \tag{7}$$

where a_i $(i = 1, 2, 3)$ represent the vectors coincident with the cell edges whereas their magnitude represent the cell lengths.

The generalized set of elastic moduli C_{rs}, can be defined by

$$C_{rs} = \frac{\partial^2 E}{\partial q_r \partial q_s} \tag{8}$$

where q_r $(r = 1, 2, \ldots, 6)$ are generalized co-ordinates. With the help of eqs (3) and (8), we obtain the expressions for the set of new moduli C_{rs}^N. The new set of elastic moduli thus obtained are

$$\begin{aligned} C_{iiii}^N &= \tfrac{1}{4}(1+k)^2 a_0^4 l_i^4 \left(\frac{\lambda_{ii}}{\lambda_{ii}+k}\right)^2 \frac{\partial^2 E}{(\partial r^2)^2} \\ &\quad + \tfrac{1}{2}k(1+k)^2 a_0^2 \frac{l_i^2}{(\lambda_{ii}+k)^3} \frac{\partial E}{\partial r^2} \end{aligned} \tag{9a}$$

$$C_{iijj}^N = \tfrac{1}{4}(1+k)^2 a_0^4 l_i^2 l_j^2 \frac{\lambda_{ii}\lambda_{jj}}{(\lambda_{ii}+k)(\lambda_{jj}+k)} \frac{\partial^2 E}{(\partial r^2)^2} \tag{9b}$$

$$\begin{aligned} C_{ijij}^N &= \tfrac{1}{4}(1+k)^2 a_0^4 l_i^2 l_j^2 \frac{(\lambda_{ii}+\lambda_{jj})^2}{(\lambda_{ii}+\lambda_{jj}+2k)^2} \frac{\partial^2 E}{(\partial r^2)^2} \\ &\quad + \tfrac{1}{2} a_0^2 \frac{k(1+k)^2}{(\lambda_{ii}+\lambda_{jj}+2k)^2} \left[\frac{l_i^2}{\lambda_{ii}+k} + \frac{l_j^2}{\lambda_{jj}+k}\right] \frac{\partial E}{\partial r^2} \end{aligned} \tag{9c}$$

$(i, j = 1, 2, 3;\ i \neq j)$.

These elastic moduli C_{rs}^N have the rotational symmetry.

The derivation of eqs (9) is given in Appendix A. For $k=0$, eqs (9) reduce to

$$C_{iiii}^G = \tfrac{1}{4} a_0^4 l_i^4 \frac{\partial^2 E}{(\partial r^2)^2} \tag{10a}$$

$$C^G_{iijj} = \tfrac{1}{4} a_0^4 l_i^2 l_j^2 \frac{\partial^2 E}{(\partial r^2)^2} \tag{10b}$$

$$C^G_{ijij} = \tfrac{1}{4} a_0^4 l_i^2 l_j^2 \frac{\partial^2 E}{(\partial r^2)^2} \quad (i,j = 1,2,3;\ i \neq j) \tag{10c}$$

which represents the set of Green moduli, C^G_{rs}, used by Born-School.

Again if we put $k = \infty$ in eqs (9), we find that the C^N_{rs} generate the stretch moduli, C^S_{rs}, a choice of Macmillan and Kelly (1972a,b, 1973).

$$C^S_{iiii} = \lambda_{ii}^2 C^G_{iiii} + \tfrac{1}{2} a_0^2 l_i^2 \frac{\partial E}{\partial r^2} \tag{11a}$$

$$C^S_{iijj} = \lambda_{ii}\lambda_{jj} C^G_{iijj} \tag{11b}$$

$$C^S_{ijij} = \tfrac{1}{4}(\lambda_{ii} + \lambda_{jj})^2 C^G_{ijij} + \tfrac{1}{4}(p^G_{ii} + p^G_{jj}) \tag{11c}$$

$$(i,j = 1,2,3; i \neq j)$$

where $p^G_{ii} = \partial E/\partial q^G_i$.

Thus we see that in special cases the C^N_{rs} can lead to the G-moduli, C^G_{rs}, the S-moduli, C^S_{rs}. Moreover, the set of new moduli, C^N_{rs}, is capable of reproducing any desired set of elastic moduli depending upon the choice of k.

3. Comparison theorem

Following Hill and Milstein (1977) we obtain the differences between S-strength and N-strength of the deformed crystal

$$S - N = p^N_r \left(\frac{\partial^2 q^N_r}{\partial q^s_u \partial q^s_v} \right) \delta q^s_u \delta q^s_v \quad (r,u,v = 1,2,\ldots,6) \tag{12}$$

which with the help of eqs (3) and (6) yield of cubic crystal deformed to orthorhombic structure

$$\begin{aligned} S - N = {} & p^G_1 \left[\frac{\lambda_{11}}{\lambda_{11}+k} \{(\delta\lambda_{11})^2 + (\delta\lambda_{13})^2 + (\delta\lambda_{12})^2\} \right] + \cdots + \cdots \\ & + 2p^G_4 \left[\frac{(\lambda_{22}+\lambda_{33})}{(\lambda_{22}+\lambda_{33}+2k)} \{(\lambda_{22}+\lambda_{33})\delta\lambda_{23} + \delta\lambda_{12}\delta\lambda_{13}\} \right]. \\ & + \cdots + \cdots \end{aligned} \tag{13}$$

Hill and Milstein (1972) calculated the values of $S - G$

$$\begin{aligned} S - G = {} & p^G_1 [(\delta\lambda_{11})^2 + (\delta\lambda_{13})^2 + (\delta\lambda_{12})^2] + \cdots + \cdots \\ & + 2p^G_4 [(\lambda_{22}+\lambda_{33})\delta\lambda_{23} + \delta\lambda_{13}\delta\lambda_{12}] + \cdots + \cdots \end{aligned} \tag{14}$$

From (13) and (14), we obtain

$$G - N = p^G_1 \left[\{(\delta\lambda_{11})^2 + (\delta\lambda_{13})^2 + (\delta\lambda_{12})^2\} \left(\frac{\lambda_{11}}{\lambda_{11}+k} - 1 \right) \right] + \cdots + \cdots + \cdots$$

$$+ 2p_4^G\left[\left\{\frac{(\lambda_{22}+\lambda_{33})}{(\lambda_{22}+\lambda_{33}+2k)}-1\right\}\{(\lambda_{22}+\lambda_{33})\delta\lambda_{23}+\delta\lambda_{13}\delta\lambda_{12}\}\right]. \tag{15}$$

The simple relations (13), (14) and (15) enable the stability to be compared via the respective convexity criteria. On the considered path of deformation, for positive loads, i.e. $p_1, p_2, p_3 \geqslant 0$ and $k > 0$, we find that the various strengths could be compared as

$$S \geqslant N \geqslant G \tag{16}$$

when $k < 0$ and p_1, p_2, $p_3 \geqslant 0$, we obtain

$$S \geqslant G \geqslant N \tag{17}$$

and when $k = -\lambda_1$ or $k = \lambda_2$ or $k = -\lambda_3$, we obtain

$$G - N = \infty; \quad N = -\infty \tag{18}$$

when p_1, p_2, $p_3 \leqslant 0$ and $k > 0$, we find that

$$G \geqslant S \geqslant N \tag{19}$$

when $k < 0$ and p_1, p_2, $p_3 \leqslant 0$

$$N \geqslant G \geqslant S \tag{20}$$

and when $k = -\lambda_1$ or $k = -\lambda_2$ or $k = -\lambda_3$, we have

$$G - N = -\infty; \quad N = \infty \tag{21}$$

4. Application to BCC iron under hydrostatic stresses

As a specific example we study the mechanics of *bcc* iron subjected to hydrostatic compressive and tensile stresses. The Morse potential as well as the generalized Morse potentials have failed to represent the behaviour of *bcc* iron. However, a recent study (Thakur 1985) has revealed that the generalized logrithmic potential is capable of representing the mechanical behaviour of iron and other *bcc* metals

$$\phi(r) = -\frac{\lambda}{r^3} + B\ln\left(1 + \frac{P}{r^{20}}\right) \tag{22}$$

where A, B and P are potential parameters taken for present computation from Thakur (1985).

We have computed the values of internal energy, stresses, cell lengths, bulk modulus, K, shear moduli μ and μ' and the elastic moduli C_{rs} (Green, stretch and the generalized moduli) of *bcc* iron as a function of lattice deformation. In the stress-free state we obtain for bcc iron

$K = 1{\cdot}69$ mega bar

$\mu = 0{\cdot}51$ mega bar

$\mu' = 1{\cdot}35$ mega bar

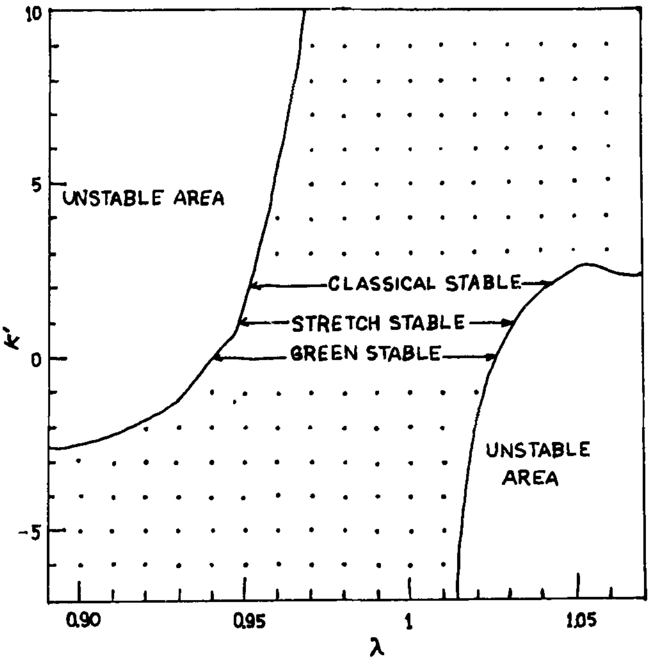

Figure 1. Stable range of iron subjected to hydrostatic compressive and tensile stresses according to present generalized moduli together with the conventional stable ranges (viz. classical, green and stretch).

various computational techniques are described in the literature (Thakur 1982a, b, 1985). The present generalized moduli C_{rs}^N are computed as a function of reduced variable

$$K' = \frac{k}{1+k}$$

for a particular lattice deformation.

The stable ranges thus obtained according to the Born criteria is presented in figure 1. Figure 1 also presents the stable ranges obtained from the Green moduli, stretch moduli as also the classical stable range (Thakur 1985).

The stable range obtained from the new strain variables (eq. 1) varies under tension from cell length of $a = 2{\cdot}905$Å to $a = 3{\cdot}06$Å and under compression from $a = 2{\cdot}61$Å to $a = 2{\cdot}767$Å depending upon the choice of strain parameter k'. The values of cell lengths and pressure at the onset of lattice instability (Green, stretch and classical instabilities) for iron under the present study are listed in table 1 together with the values of strain parameter k', for which the generalized results are equivalent to the conventional ones. Figure 1 and table 1 indicate that all the conventional ranges could be generated as the specific cases of our generalized results. Figure 1 also shows that the stable range of *bcc* iron under hydrostatic compression is limited by all the conventional variables. However, in actual practice, iron is stable under hydrostatic compression up to considerably large strain, which is possible only if we consider our generalized variables with $K' < -2{\cdot}6$ (Figure 1).

Table 1. Cell length (a in Å) and pressure (p in Mbar) at the onset of lattice instability (G-, S-, and N-stabilities) for iron under hydrostatic stresses together with the values of k' for which generalized results are equivalent to the conventional ones.

Stability type	Stability failure under compression			Stability failure under tension			k'
	a	p	Cause	a	p	Cause	
Classical	2·720	0·253	$\mu' = 0$	2·980	−0·205	$\mu = 0$	2
Green	2·690	0·308	$C_{44} = 0$	2·935	−0·129	$C_{11} = C_{12}$	0
Stretch	2·714	0·265	$C_{44} = 0$	2·950	−0·156	$C_{11} = C_{12}$	1

5. Third order elastic constants

In the past few decades the third order elastic constant (TOEC) of crystals has been a topic of extensive study (Birch 1947; Nranyan 1964; Thurston and Brugger 1964) and plays an important role in solid state physics. Brugger (1964) presented a general thermodynamic definition of higher order elastic constant. The most general definition for elastic constants of the nth order is

$$C_{rst\ldots} = \frac{\partial^n E}{\partial q_r \partial q_s \partial q_t \ldots}; \quad n \geqslant 2 \tag{23}$$

where q_r ($r = 1, 2, \ldots, 6$) are the generalized co-ordinates defined earlier, E is the internal energy per unit reference volume and may be expressed as a function of q_r.

From (23) the third order elastic constant, C_{rst}, can be defined by

$$C_{rst} = \frac{\partial^3 E}{\partial q_r \partial q_s \partial q_t}. \tag{24}$$

Taking q_r^N, the new set of generalized variables (eq. 1) for q_r in (24), we generate the expressions for the third order elastic constants, C_{rst}^N,

$$C_{rrr}^N = \tfrac{1}{8} a_0^6 l_r^6 (1+k)^3 \left(\frac{\lambda_r}{\lambda_r + k}\right)^3 \frac{\partial^3 E}{(\partial r^2)^3} + \tfrac{3}{4} a_0^4 l_r^4 \frac{k(1+k)^3 \lambda_r}{(\lambda_r + k)} \frac{\partial^2 E}{(\partial r^2)^2}$$
$$- \tfrac{3}{2} k(1+k)^3 \frac{a_0^2 l_r^2}{(\lambda_r + k)^5} \frac{\partial E}{\partial r^2} \quad (r = 1, 2, 3) \tag{25a}$$

$$C_{rrs}^N = \tfrac{1}{8} a_0^6 l_r^4 l_s^2 (1+k)^3 \frac{\lambda_r^2 \lambda_s}{(\lambda_r + k)^2 (\lambda_s + k)} \frac{\partial^3 E}{(\partial r^2)^3}$$
$$+ \tfrac{1}{4} k l_r^2 l_s^2 a_0^4 (1+k)^3 \frac{\lambda_s}{(\lambda_r + k)^3 (\lambda_s + k)} \frac{\partial^2 E}{(\partial r^2)^2} \quad (r, s = 1, 2, 3;\ r \neq s) \tag{25b}$$

$$C_{rst}^N = \tfrac{1}{8} a_0^6 l_r^2 l_s^2 l_t^2 (1+k)^3 \frac{\lambda_r \lambda_s \lambda_t}{(\lambda_r + k)(\lambda_s + k)(\lambda_t + k)} \frac{\partial^3 E}{(\partial r^2)^3}$$
$$(r, s, t = 1, 2, 3;\ r \neq s \neq t) \tag{25c}$$

$$C_{144}^N = \tfrac{1}{8}a_0^6 l_1^2 l_2^2 l_3^2 (1+k)^3 \frac{\lambda_1(\lambda_2+\lambda_3)^2}{(\lambda_2+\lambda_3+2k)^2(\lambda_1+k)} \frac{\partial^3 E}{(\partial r^2)^3}$$

$$+\tfrac{1}{4}a_0^4 l_1^2 \frac{k(1+k)^3\lambda_1}{(\lambda_1+k)(\lambda_2+\lambda_3+2k)^2}\left\{\frac{l_2^2}{(\lambda_2+k)}+\frac{l_3^2}{(\lambda_3+k)}\right\}\frac{\partial^2 E}{(\partial r^2)^2} \quad (25d)$$

$$C_{166}^N = \tfrac{1}{8}a_0^6 l_1^4 l_2^2 (1+k)^3 \frac{\lambda_1(\lambda_1+\lambda_2)^2}{(\lambda_1+k)(\lambda_1+\lambda_2+2k)^2} \frac{\partial^3 E}{(\partial r^2)^3}$$

$$+\tfrac{1}{4}a_0^4 l_1^2 \frac{k(1+k)^3\lambda_1}{(\lambda_1+k)(\lambda_1+\lambda_2+2k)^2}\left\{\frac{l_1^2}{(\lambda_1+k)}+\frac{l_2^2}{(\lambda_2+k)}\right\}\frac{\partial^2 E}{(\partial r^2)^2}$$

$$-k(1+k)^3\left[\frac{2(\lambda_1+k)+(\lambda_1+\lambda_2+2k)}{(\lambda_1+k)^3(\lambda_1+\lambda_2+2k)^3}\right]p_{11}^G \quad (25e)$$

The derivation of eqs (25) is given in Appendix A2.
Taking $k=0$ in (25), we obtain the third order Green moduli

$$C_{rrr}^G = \tfrac{1}{8}a_0^6 l_r^6 \frac{\partial^3 E}{(\partial r^2)^3} \quad (r=1,2,3) \quad (26a)$$

$$C_{rrs}^G = \tfrac{1}{8}a_0^6 l_r^4 l_s^2 \frac{\partial^3 E}{(\partial r^2)^3} \quad (r,s=1,2,3;\ r\neq s) \quad (26b)$$

$$C_{rst}^G = \tfrac{1}{8}a_0^6 l_r^2 l_s^2 l_t^2 \frac{\partial^3 E}{(\partial r^2)^3} \quad (r,s,t=1,2,3;\ r\neq s\neq t) \quad (26c)$$

$$C_{144}^G = \tfrac{1}{8}a_0^6 l_1^2 l_2^2 l_3^2 \frac{\partial^3 E}{(\partial r^2)^3} \quad (26d)$$

$$C_{166}^G = \tfrac{1}{8}a_0^6 l_1^4 l_2^2 \frac{\partial^3 E}{(\partial r^2)^3}. \quad (26e)$$

And for $k=\infty$, (25) reduces to the third order stretch moduli

$$C_{rrr}^S = 3\lambda_r C_{rr}^G + \lambda_r^3 C_{rrr}^G \quad (r=1,2,3) \quad (27a)$$

$$C_{rrs}^S = \lambda_s C_{rs}^G + \lambda_r^2\lambda_s C_{rrs}^G \quad (r,s=1,2,3;\ r\neq s) \quad (27b)$$

$$C_{rst}^S = \lambda_r\lambda_s\lambda_t C_{rst}^G \quad (r,s,t=1,2,3;\ r\neq s\neq t) \quad (27c)$$

$$C_{144}^S = \tfrac{1}{4}\lambda_1[C_{12}^G + C_{13}^G + (\lambda_2+\lambda_3)^2 C_{144}^G] \quad (27d)$$

$$C_{166}^S = \tfrac{1}{6}\lambda_1[C_{11}^G + C_{12}^G + (\lambda_1+\lambda_2)^2 C_{166}^G]. \quad (27e)$$

Thus we see that in special cases the C_{rst}^N can lead to the G-moduli, C_{rst}^G, and the S- moduli, C_{rst}^S. Moreover, the set of new moduli C_{rst}^N is capable of reproducing any desired set of third order elastic moduli depending upon the choice of k.

6. Energy convexity

The stability criterion was first initiated by Born (1940) which is popularly known as the Born stability condition. It may be taken to be equivalent to the condition that the internal energy function 'E' be locally strictly convex in the arguments. In a deformed state the positive definiteness of the quadratic terms in Taylor's expansion of the internal energy

$$\delta E = p_r \delta q_r + \tfrac{1}{2} C_{rs} \delta q_r \delta q_s + \tfrac{1}{6} C_{rst} \delta q_r \delta q_s \delta q_t + \cdots,$$
$$(r, s, t = 1, 2, \ldots 6, \text{ summation convention}) \tag{28}$$

is taken as the stability criterion.

Under the combined effect of second degree and third degree terms, the stability criterion may routinely be expressed as

$$\left(\sum_{r,s=1}^{6} \tfrac{1}{2} C_{rs} \delta q_r \delta q_s + \sum_{r,s,t=1}^{6} \tfrac{1}{6} C_{rst} \delta q_r \delta q_s \delta q_t \right) > 0. \tag{29}$$

For cubic crystal under lod, deformed to orthorhombic structure, we obtain

$$X^S - X^N = \sum_{i,j,k_1=1}^{3} \frac{\lambda_{ii}}{\lambda_{ii} + k} p_{ii}^G \{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\} \quad i \neq j \neq k_1 \tag{30}$$

which for $k = 0$ reduces to

$$X^S - X^G = \sum_{i,j,k_1=1}^{3} p_{ii}^G \{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\} \quad i \neq j \neq k_1 \tag{31}$$

where N-stability becomes equal to the G-stability. On the other hand for $k = \infty$, right hand side of (30) vanishes and clearly N-strength and S-strength becomes equal to each other.

Let us write the transformation rule for third order elastic constants as

$$\begin{aligned} & C_{uvw}^S \delta q_u^S \delta q_v^S \delta q_w^S - C_{rst}^N \delta q_r^N \delta q_s^N \delta q_t^N \\ &= C_{rs}^N \left[\frac{\partial^2 q_r^N}{\partial q_u^S \partial q_w^S} \frac{\partial q_s^N}{\partial q_v^S} + \frac{\partial^2 q_r^N}{\partial q_u^S \partial q_v^S} \frac{\partial q_s^N}{\partial q_w^S} + \frac{\partial^2 q_s^N}{\partial q_v^S \partial q_w^S} \frac{\partial q_r^N}{\partial q_u^S} \right] \\ &\quad \times \delta q_u^S \delta q_v^S \delta q_w^S + p_r^N \frac{\partial^3 q_r^N}{\partial q_u^S \partial q_v^S \partial q_w^S} \delta q_u^S \delta q_v^S \delta q_w^S \end{aligned} \tag{32}$$

with the help of (3) and (6), one can calculate the partial derivatives of the right hand side of (32)

$$\begin{aligned} X^S - X^N = \frac{3}{(1+k)^2} \sum_{i,j,k_1=1}^{3} & \{ C_{iiii}^N (\lambda_{ii} + k) \delta\lambda_{ii} + C_{iijj}^N (\lambda_{jj} + k) \delta\lambda_{jj} \\ & + C_{iik_1k_1}^N (\lambda_{k_1k_1} + k) \delta\lambda_{k_1k_1} \} \{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\} \\ & i \neq j \neq k_1 \end{aligned} \tag{33}$$

where X^S and X^N denotes, respectively, the quantities C_{uvw}^S δq_u^S $\delta q_v^S \delta q_w^S$ and C_{rst}^N $\delta q_r^N \delta q_s^N \delta q_t^N$.

From (29) and (33) under considered path of loading

$$S - N = \sum_{i,j,k_1=1}^{3} \frac{1}{2(1+k)} \left[\left\{ p_{ii}^N + C_{iiii}^N \frac{(\lambda_{ii} + k)}{(1+k)} \delta\lambda_{ii} \right. \right.$$

$$+ C^N_{iijj}\frac{(\lambda_{jj}+k)}{(1+k)}\delta\lambda_{jj} + C^N_{iik_1k_1}\frac{(\lambda_{k_1k_1}+k)}{(1+k)}\delta\lambda_{k_1k_1}\Big\}$$

$$\{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\}\Big]\, i \neq j \neq k_1 \tag{34}$$

where S and N denotes respectively, the crystal strengths relative to the stretch and new variables, when up to third degree terms in the internal energy expansion, (28), is taken into account. If we put the values of p_{ii} and C^N_{rs} in terms of G-moduli, we reproduce the result in terms of Green's and the stretch variables

$$S - N = \sum_{i,j,k_1=1}^{3} \frac{1}{2(\lambda_{ii}+k)}\left[\left\{\lambda_{ii} + \frac{k(1+k)}{(\lambda_{ii}+k)^2}\right\} p^G_{ii} + C^G_{iiii}(\lambda_{ii})^2\delta\lambda_{ii} + C_{iijj}\lambda_{ii}\lambda_{jj}\delta\lambda_{jj} + C_{iik_1k_1}\lambda_{ii}\lambda_{k_1k_1}\delta\lambda_{k_1k_1}\right]\{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\} \quad i \neq j \neq k_1 \tag{35}$$

which for $k = 0$ reduces to

$$S - G = \sum_{i,j,k_1=1}^{3} \tfrac{1}{2}[\{p^G_{ii} + C^G_{iiii}\lambda_{ii}\delta\lambda_{ii} + C^G_{iijj}\lambda_{jj}\delta\lambda_{jj} + C_{iik_1k_1}\lambda_{k_1k_1}\delta\lambda_{k_1k_1}\} \times \{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\} \quad i \neq j \neq k_1 \tag{36}$$

In this case N-strength becomes equal to G-strength. For $K = \infty$, the right hand side of (35) becomes zero and hence, the N-strength becomes equal to S-strength. Equations (35) and (36) together lead to

$$N - G = \sum_{i,j,k_1=1}^{3}\left[\left\{1 - \frac{\lambda_{ii}}{\lambda_{ii}+k} - \frac{k(1+k)}{(\lambda_{ii}+k)^3}\right\} p^G_{ii} + \{C^G_{iiii}\lambda_{ii}\delta\lambda_{ii} + C^G_{iijj}\lambda_{jj}\delta\lambda_{jj} + C^G_{iik_1k_1}\lambda_{k_1k_1}\delta\lambda_{k_1k_1}\}\left(1 - \frac{\lambda_{ii}}{\lambda_{ii}+k}\right)\right]\{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\} \quad i \neq j \neq k_1 \tag{37}$$

which vanishes for $k = 0$, reduces to (36) for $k = \infty$ and since in these cases N-strength becomes equal to G-strength and S-strength respectively. We consider the case in which the reference cell is a unit cube which under load gets deformed to orthorhombic structure with cell edges parallel to the symmetry axes. Neglecting for a moment, the third order effect, we reproduce (36) as

$$S - G = \sum_{i,j,k_1=1}^{3} \tfrac{1}{2} p^G_{ii}\{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\} \quad i \neq j \neq k_1 \tag{38}$$

when only the second order terms are considered. Comparing the co-efficients of $\{(\delta\lambda_{ii})^2 + (\delta\lambda_{ij})^2 + (\delta\lambda_{ik_1})^2\}$ in (36) and (38), we have three equations of the type

$$p^G_r + C^G_{rr}\lambda_r\delta\lambda_r + C^G_{rs}\lambda_s\delta\lambda_s + C^G_{rt}\lambda_t\delta\lambda_t \geqslant p^G_r \tag{39}$$

$(r, s, t = 1, 2, 3;\ r \neq s \neq t)$; where (ii)$\to r$, $(jj)\to s$, $(k_1k_1)\to t$

when the crystal is subjected to a uniaxial deformation, let us examine (39). In this particular mode of loading the axial stretch $\lambda_r \neq 1$ whereas the transverse stretches $\lambda_s = \lambda_t = 1$

$$\text{i.e. } \delta\lambda_r \neq 0, \quad \delta\lambda_s = \delta\lambda_t = 0 \quad (r, s, t = 1, 2, 3;\ r \neq s \neq t)$$

Tensile stresses, $\lambda_r > 1$

In this state of loading the existing term $C^G_{rr}\lambda_r\delta\lambda_r$ in (39) is greater than zero, since C^G_{rr} is itself positive and (38) implies that

$$p^G_r + C^G_{rr}\lambda_r\delta\lambda_r > p^G_r.$$

Hence

$$(S - G) > (S' - G').$$

Moreover, in the current state of positive stress, (36) implies that S-strength is greater than G-strength.

Compressive stresses

For compressive stress $\lambda_r < 1$, exactly reverse situation arises since $\delta\lambda_r$ makes the term $C^G_{rr}\lambda_r\delta\lambda_r$ less than zero.

With similar arguments (36) implies that S-strength is less than G-strength in negative loading.

Plane dilation

In plane stress where axial stretch $\lambda_r = 1$ and transverse stretches $\lambda_s = \lambda_t \neq 1$, i.e. $\delta\lambda_r = 0$ and $\delta\lambda_S = \delta\lambda_t \neq 0$. $(r, s, t = 1, 2, 3;\ r \neq s \neq t)$.

In the first case of plane dilation, when $\lambda_r = 1$ and $\lambda_s = \lambda_t > 1$ and the SOEC C^G_{rs} and C^G_{rt} are such that the quantities $(C^G_{rs}\lambda_s\delta\lambda_s + C^G_{rt}\lambda_t\delta\lambda_t)$ in (39) becomes greater than zero, then S-strength will be greater than the G-strength.

Plane contraction

In the second case of plane contraction, when $\lambda_r = 1$ and $\lambda_s = \lambda_t < 1$ and the SOEC C^G_{rs} and C^G_{rt} are such that the quantities $(C^G_{rs}\lambda_s\delta\lambda_s + C^G_{rt}\lambda_t\delta\lambda_t)$ in (39) becomes less than zero, then S-strength will be less than G-strength.

Under the same loading paths as illustrated above and with the same reference state one may readily compare the relative stabilities in S-variables and N-variables (or in G-variables and N-variables) as in (35) or (38).

7. Summary and conclusion

In this paper a new generalized set of strain variables, q^N_r, has been used for the determination of the new set of second order elastic moduli, C^N_{rs}, and third order elastic moduli, C^N_{rst}. The new generalized set of strain variables q^N_r, and the new set of elastic moduli, C^N_{rs} and C^N_{rst}, reduce respectively to Green's co-ordinate, q^G_r, and

Green's moduli, C^G_{rs} and C^G_{rst}, after taking $k=0$ in (3), (9) and (25) respectively. After taking $k=\infty$ in these equations, the q^N_r, C^N_{rs} and C^N_{rst} reduce, respectively, to the stretch co-ordinates, q^S_r and the stretch moduli C^S_{rs} and C^S_{rst}. Thus the new co-ordinates q^N_r and new elastic moduli C^N_{rs} and C^N_{rst} are the generalization of the corresponding terms derived from Green and stretch variables.

Also the requisite components obtained from the new co-ordinates, have enabled comparision of theoretical strength of the crystals according to the present scale function with the conventional Green-strength used by Born-School, stretch-strength used by Macmillan and Kelly, for cubic crystals deformed to orthorhombic structure.

From comparision, we conclude that

$$G\text{-strength} \leqslant N\text{-strength} \leqslant S\text{-strength}$$

when load is positive definite and k is positive. But when load is positive and k is negative, it is found that

$$S\text{-strength} \geqslant G\text{-strength} \geqslant N\text{-strength}$$

and when $k=-\lambda_1$, or $k=-\lambda_2$, or $k=-\lambda_3$ and $p_1, p_2, p_3 \geqslant 0$ then N-strength $=-\infty$. But when load is negative, i.e. p_1, p_2, $p_3 \leqslant 0$, outstability condition changes to

(i) $G \geqslant S \geqslant N$, for $k>0$
(ii) $N \geqslant G \geqslant S$, for $k<0$

and (iii) when $k=-\lambda_1$, or $k=-\lambda_2$ or $k=-\lambda_3$ and p_1, p_2, $p_3 \leqslant 0$ then N-strength $=+\infty$.

Further we have estimated lattice stability by comparing directly the convexity criteria relative to various choices of strain measures (G-variables, S-variables and N-variables) when up to third degree terms in the energy expansion are considered.

Finally, we present the computational results for a *bcc* iron subjected to hydrostatic compressive and tensile stresses according to the new set of elastic moduli. The results are summarised in figure 1 and table 1 which indicate that all the conventional stable ranges could be generated as the specific cases of our generalized results. However, the conventional stable ranges fail to represent the state of hydrostatic compression of iron, where only the present study can generate realistic results.

Appendix A

Expressions for C^N_{rs}, eq (9), can be derived using (3), (4), (7) and (8). For example, a detailed derivation of the moduli C^N_{11}, C^N_{12} and C^N_{44} is given here. By the definition (8), we have

$$C^N_{11} = \frac{\partial^2 E}{\partial q^N_1 \partial q^N_1} = \frac{\partial}{\partial q^N_1}\left(\frac{\partial E}{\partial q^N_1}\right) = \frac{\partial}{\partial q^N_1}\left(\frac{\partial E}{\partial r^2}\frac{\partial r^2}{\partial a_1}\frac{\partial a_1}{\partial q^N_1}\right). \tag{A1}$$

Now,

$$\frac{\partial r^2}{\partial a_1} = \tfrac{1}{2} l_1^2 a_1$$

and

$$\frac{\partial q_1^N}{\partial a_1} = \frac{1}{1+k}\left(\frac{\lambda_1 + k}{a_0}\right) \tag{A2}$$

where

$$\lambda_1 = a_1/a_0. \tag{A3}$$

Hence from (A1), (A2) and (A3) we have

$$C_{11}^N = \tfrac{1}{4} l_1^4 a_0^4 (1+k)^2 \left(\frac{\lambda_1}{\lambda_1 + k}\right)^2 \frac{\partial^2 E}{(\partial r^2)^2} + \tfrac{1}{2} k(1+k)^2 \frac{a_0^2 l_1^2}{(\lambda_1 + k)^3} \frac{\partial E}{\partial r^2}. \tag{A4}$$

Similarly we obtain

$$C_{12}^N = \tfrac{1}{4} a_0^4 (1+k)^2 l_1^2 l_2^2 \frac{\lambda_1 \lambda_2}{(\lambda_1 + k)(\lambda_2 + k)} \frac{\partial^2 E}{(\partial r^2)^2}. \tag{A5}$$

Next for C_{44}^N we have from (8)

$$C_{44}^N = \frac{\partial^2 E}{\partial q_4^N \partial q_4^N} = \frac{\partial}{\partial q_4^N}\left(\frac{\partial E}{\partial \lambda_4}\frac{\partial \lambda_4}{\partial q_4^N}\right) = \frac{\partial}{\partial q_4^N}\left(\frac{\partial E}{\partial \lambda_4}\frac{(1+k)}{(\lambda_2 + \lambda_3 + 2k)}\right)$$

or

$$C_{44}^N = \tfrac{1}{4} a_0^4 l_2^2 l_3^2 (1+k)^2 \frac{(\lambda_2 + \lambda_3)^2}{(\lambda_2 + \lambda_3 + 2k)^2} \frac{\partial^2 E}{(\partial r^2)^2} + \tfrac{1}{2} k(1+k)^2 \frac{a_0^2}{(\lambda_2 + \lambda_3 + 2k)^2}\left[\frac{l_2^2}{(\lambda_2 + k)} + \frac{l_3^2}{(\lambda_3 + k)}\right]\frac{\partial E}{\partial r^2} \tag{A6}$$

Appendix B

Expressions for C_{rst}^N, (25), can be derived using (3), (4), (7), (8) and (9). For example a detail derivation of the C_{111}^N, C_{112}^N, C_{123}^N, C_{144}^N and C_{166}^N are given here.

By the definition (25) we have

$$\begin{aligned} C_{111}^N &= \frac{\partial^3 E}{\partial q_1^N \partial q_1^N \partial q_1^N} = \frac{\partial}{\partial q_1^N}\left(\frac{\partial^2 E}{(\partial q_1^N)^2}\right) \\ &= \frac{\partial}{\partial q_1^N}\left[\tfrac{1}{4}(1+k)^2 a_0^4 l_1^4 \left(\frac{\lambda_1}{\lambda_1 + k}\right)^2 \frac{\partial^2 E}{(\partial r^2)^2} \right. \\ &\quad \left. + \tfrac{1}{2} k(1+k)^2 \frac{a_0^2 l_1^2}{(\lambda_1 + k)^3} \frac{\partial E}{\partial r^2}\right] \\ &= \tfrac{1}{4} a_0^4 l_1^4 (1+k)^2 \left[\left(\frac{\lambda_1}{\lambda_1 + k}\right)^2 \frac{\partial^3 E}{(\partial r^2)^3} \tfrac{1}{2} l_1^2 a_1^2 \frac{a_0(1+k)}{\lambda_1 + k} \right. \\ &\quad \left. + \frac{\partial^2 E}{(\partial r^2)^2}\left\{(\lambda_1 + k)^2 \frac{2\lambda_1}{a_0} \frac{a_0(1+k)}{(\lambda_1 + k)} - \lambda_1^2 \frac{2(\lambda_1 + k)}{a_0} \frac{a_0(1+k)}{(\lambda_1 + k)}\right\}\right] \\ &\quad + \tfrac{1}{2} k(1+k)^2 a_0^2 l_1^2 \left[\frac{1}{(\lambda_1 + k)^3} \frac{\partial^2 E}{(\partial r^2)^2} \tfrac{1}{2} l_1^2 a_1 \frac{a_0(1+k)}{(\lambda_1 + k)}\right. \end{aligned}$$

$$-\frac{3}{(\lambda_1+k)^4}\frac{1}{a_0}\frac{a_0(1+k)}{(\lambda_1+k)}\frac{\partial E}{\partial r^2}\Bigg]$$

$$=\tfrac{1}{8}a_0^6 l_1^6(1+k)^3\left(\frac{\lambda_1}{\lambda_1+k}\right)^3\frac{\partial^3 E}{(\partial r^2)^3}+\tfrac{3}{4}a_0^4 l_1^4\frac{(1+k)^3\lambda_1 k}{(\lambda_1+k)^4}\frac{\partial^2 E}{(\partial r^2)^2}$$

$$-\tfrac{3}{2}k(1+k)^3\frac{a_0^2 l_1^2}{(\lambda_1+k)^5}\frac{\partial E}{\partial r^2}.$$

For C_{112}^N, we have from (25)

$$C_{112}^N=\frac{\partial^3 E}{\partial q_1^N\partial q_1^N\partial q_2^N}=\frac{\partial}{\partial q_1^N}\left(\frac{\partial^2 E}{\partial q_1^N\partial q_2^N}\right)$$

$$=\frac{\partial}{\partial q_1^N}\left[\tfrac{1}{4}l_1^2 l_2^2 a_0^4(1+k)^2\frac{\lambda_1\lambda_2}{(\lambda_1+k)(\lambda_2+k)}\frac{\partial^2 E}{(\partial r^2)^2}\right]$$

$$=\tfrac{1}{4}a_0^4(1+k)^2 l_1^2 l_2^2\left[\frac{\lambda_1\lambda_2}{(\lambda_1+k)(\lambda_2+k)}\frac{\partial^3 E}{(\partial r^2)^3}\frac{\partial r^2}{\partial a_1}\frac{\partial a_1}{\partial q_1^N}\right.$$

$$\left.+\frac{\partial^2 E}{(\partial r^2)^2}\left\{\frac{(\lambda_1+k)(\lambda_2+k)\lambda_2/a_0\dfrac{a_0(1+k)}{(\lambda_1+k)}-\lambda_1\lambda_2(\lambda_2+k)\dfrac{a_0(1+k)}{(\lambda_1+k)}}{(\lambda_1+k)^2(\lambda_2+k)^2}\right\}\right]$$

$$=\tfrac{1}{4}a_0^4(1+k)^2 l_1^2 l_2^2\left[\frac{\lambda_1\lambda_2}{(\lambda_1+k)(\lambda_2+k)}\tfrac{1}{2}l_1^2 a_1\frac{a_0(1+k)}{\lambda_1+k}\frac{\partial^3 E}{(\partial r^2)^3}\right.$$

$$\left.+(1+k)\left\{\frac{\lambda_1\lambda_2+\lambda_2 k-\lambda_1\lambda_2}{(\lambda_1+k)^3(\lambda_2+k)}\right\}\frac{\partial^2 E}{(\partial r^2)^2}\right]$$

$$=\tfrac{1}{8}a_0^6 l_1^4 l_2^2(1+k)^3\frac{\lambda_1^2\lambda_2}{(\lambda_1+k)^2(\lambda_2+k)}\frac{\partial^3 E}{(\partial r^2)^3}$$

$$+\tfrac{1}{4}l_1^2 l_2^2 a_0^4\frac{(1+k)^3 k\lambda_2}{(\lambda_1+k)^3(\lambda_2+k)}\frac{\partial^2 E}{(\partial r^2)^2}.$$

For C_{123}^N, we have from (25)

$$C_{123}^N=\frac{\partial}{\partial q_1^N}\left(\frac{\partial^2 E}{\partial q_2^N\partial q_3^N}\right)=\frac{\partial}{\partial q_1^N}\left[\frac{1}{4}\frac{l_2^2 l_3^2 a_0^4(1+k)^2\lambda_2\lambda_3}{(\lambda_2+k)(\lambda_3+k)}\frac{\partial^2 E}{(\partial r^2)^2}\right]$$

$$=\tfrac{1}{4}a_0^4 l_2^2 l_3^2(1+k)^2\frac{\lambda_2\lambda_3}{(\lambda_2+k)(\lambda_3+k)}\tfrac{1}{2}l_1^2 a_1\frac{a_0(1+k)}{(\lambda_1+k)}\frac{\partial^3 E}{(\partial r^2)^3}$$

$$=\tfrac{1}{8}a_0^6 l_1^2 l_2^2 l_3^2(1+k)^3\frac{\lambda_1\lambda_2\lambda_3}{(\lambda_1+k)(\lambda_2+k)(\lambda_3+k)}\frac{\partial^3 E}{(\partial r^2)^2}.$$

For C_{144}^N, we have from (25)

$$C_{144}^N=\frac{\partial}{\partial q_1^N}\left(\frac{\partial^2 E}{\partial q_4^N\partial q_4^N}\right)$$

$$=\frac{\partial}{\partial q_1^N}\left[\left(\tfrac{1}{4}a_0^4 l_2^2 l_3^2(1+k)^2\left(\frac{\lambda_2+\lambda_3}{\lambda_2+\lambda_3+2k}\right)^2\frac{\partial^2 E}{(\partial r^2)^2}\right)\right.$$

$$+\tfrac{1}{2}a_0^2\frac{l_2^2k(1+k)^2}{(\lambda_2+\lambda_3+2k)^2(\lambda_2+k)}\frac{\partial E}{\partial r^2}$$

$$+\frac{1}{2}\frac{a_0^2l_3^2(1+k)^2k}{(\lambda_2+\lambda_3+2k)^2(\lambda_3+k)}\frac{\partial E}{\partial r^2}\Bigg]$$

$$=\tfrac{1}{4}a_0^4(1+k)^2l_2^2l_3^2\left[\left(\frac{\lambda_2+\lambda_3}{\lambda_2+\lambda_3+2k}\right)^2\frac{\partial^3E}{(\partial r^2)^3}\tfrac{1}{2}l_1^2a_1\frac{a_0(1+k)}{(\lambda_1+k)}+0\right]$$

$$+\tfrac{1}{2}a_0^2l_2^2k(1+k)^2\tfrac{1}{2}\left[\frac{l_1^2a_1a_0(1+k)}{(\lambda_2+\lambda_3+2k)^2(\lambda_1+k)(\lambda_2+k)}\frac{\partial^2E}{(\partial r^2)^2}\right]$$

$$+\tfrac{1}{2}a_0^2l_3^2k(1+k)^2\left[\frac{1}{2}\frac{l_1^2a_1a_0(1+k)}{(\lambda_2+\lambda_3+2k)^2(\lambda_1+k)(\lambda_3+k)}\frac{\partial^2E}{(\partial r^2)^2}\right].$$

Hence

$$C_{144}^N=\tfrac{1}{8}a_0^6l_1^2l_1^2l_3^2\frac{(1+k)^3\lambda_1(\lambda_2+\lambda_3)^2}{(\lambda_2+\lambda_3+2K)^2(\lambda_1+k)}\frac{\partial^3E}{(\partial r^2)^3}$$

$$+\tfrac{1}{4}a_0^4l_1^2\frac{k(1+k)^3\lambda_1}{(\lambda_1+k)(\lambda_2+\lambda_3+2k)^2}\left[\frac{l_2^2}{\lambda_2+k}+\frac{l_3^2}{\lambda_3+k}\right]\frac{\partial^2E}{(\partial r^2)^2}.$$

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