Ideal Strength and Intrinsic Ductility in Metals and Alloys From Second and Third Order Elastic Constants

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I. STRAIN ENERGY DENSITY: FORAMLISM AND RESULTS

A. General expressions

Consider the mapping between the reference and current configuration of a continuum solid. In the reference configuration, a particle occupies a point $\boldsymbol{p}$ with spatial coordinates $\boldsymbol{X} = X_1\boldsymbol{e}_1 + X_2\boldsymbol{e}_2 + X_3\boldsymbol{e}_3$, where e_1, e_2, e_3 is a Cartesian reference triad and X_1, X_2, X_3 are the reference coordinates. Upon deformation of the body, the point originally at $\boldsymbol{X}$ is translated by the displacement vector $\boldsymbol{u}\left(X_1, X_2, X_3\right)$ to its final coordinates $\boldsymbol{x}\left(X_1, X_2, X_3\right)$, see Eq. 1 .

$$\boldsymbol{x}\left(X_1, X_2, X_3\right) = \boldsymbol{u}\left(X_1, X_2, X_3\right) + \boldsymbol{X}\left(X_1, X_2, X_3\right) \tag{1}$$

Based on this description, a deformation gradient is formulated as in Eq. 2. The Green-Lagrange strain tensor $\boldsymbol{\eta}$ then follows from $\boldsymbol{F}$ as shown in Eq. 3, where $\boldsymbol{I}$ denotes the identity matrix.

$$\boldsymbol{F} = \frac{\partial x_i}{\partial X_j} \tag{2}$$

$$\boldsymbol{\eta} = \frac{1}{2}\left(\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}\right) \tag{3}$$

With the notation now established, the strain energy density can be expanded in terms of the second-order elastic constants (SOEC's), third-order elastic constants (TOEC's) and the Green-Lagrange strain as in Eq. 4, where ρ_0 represents the mass density in the undeformed state and the terms η_i represent the components of the tensor defined in Eq. 3. The symmetry of the SOEC's and TOEC's will be applied in the expansions, which simplifies the resulting expressions considerably.

$$\rho_0 E\left(\boldsymbol{\eta}\right) = \frac{1}{2!}\sum_{i,j=1}^{6} C_{ij}\eta_i\eta_j + \frac{1}{3!}\sum_{i,j,k=1}^{6} C_{ijk}\eta_i\eta_j\eta_k + \ldots \tag{4}$$

In this section, it is assumed that strain control is applied along the c-axis of the crystal. To make this more explicit, we employ the notation $\xi = \eta_3$ in the following sections.

B. Cubic crystal system

We consider a cubic material that is loaded along the c-axis by a Green Lagrangian strain denoted by ξ. Initially, we allow for additional strains denoted by $\eta_1, \eta_2, \eta_4, \eta_5, \eta_6$. Consider an expansion of the strain energy density up to and including SOEC's. When the symmetry of the SOEC's is invoked, the expression in Eq. 5 is obtained.

$$\rho_0 E\left(\boldsymbol{\eta}\right) = C_{11}\frac{\eta_1^2}{2} + C_{11}\frac{\eta_2^2}{2} + C_{33}\frac{\xi^2}{2} + C_{44}\frac{\eta_4^2}{2} + C_{44}\frac{\eta_5^2}{2} + C_{44}\frac{\eta_6^2}{2} + C_{12}\eta_1\eta_2 + C_{12}\xi\eta_2 + C_{12}\eta_1\xi \tag{5}$$

Eq. 5 generally suffices for small strains. For larger strains, a higher-order expansion of the strain energy density involving TOEC's is required, as shown in Eq. 6, where the terms P_i are given in Eqs. 7.

$$\rho_0 E\left(\boldsymbol{\eta}\right) = C_{11}P_{1c} + C_{44}P_{2c} + C_{12}P_{3c} + C_{111}P_{4c} + C_{112}P_{5c} + C_{123}P_{6c} + C_{144}P_{7c} + C_{155}P_{8c} + C_{456}P_{9c} \tag{6}$$

$$P_{1c} = \frac{\eta_1^2}{2} + \frac{\eta_2^2}{2} + \frac{\xi^2}{2}, \tag{7a}$$

$$P_{2c} = \frac{\eta_4^2}{2} + \frac{\eta_5^2}{2} + \frac{\eta_6^2}{2}, \tag{7b}$$

$$P_{3c} = \eta_1\eta_2 + \eta_2\xi + \eta_1\xi, \tag{7c}$$

$$P_{4c} = \frac{1}{6}\left(\eta_1^3 + \eta_2^3 + \xi^3\right), \tag{7d}$$

$$P_{5c} = \frac{1}{2}\left(\eta_2\eta_1^2 + \xi\eta_1^2 + \eta_2^2\eta_1 + \xi^2\eta_1 + \eta_2\xi^2 + \eta_2^2\xi\right), \tag{7e}$$

$$P_{6c} = \eta_1\eta_2\xi, \tag{7f}$$

$$P_{7c} = \frac{1}{2}\left(\eta_1\eta_4^2 + \eta_2\eta_5^2 + \xi\eta_6^2\right), \tag{7g}$$

$$P_{8c} = \frac{1}{2}\left(\eta_2\eta_4^2 + \xi\eta_4^2 + \eta_1\eta_5^2 + \xi\eta_5^2 + \eta_1\eta_6^2 + \eta_2\eta_6^2\right), \tag{7h}$$

$$P_{9c} = \eta_4\eta_5\eta_6 \tag{7i}$$

C. Hexagonal crystal system

Consider an imposed strain ξ along the c-axis of an HCP-metal, in addition to strains denoted by $\eta_1, \eta_2, \eta_4, \eta_5, \eta_6$. Consider first the expansion of Eq. 4, retaining only terms up to and including the SOEC's (hence, ignoring the TOEC's for now). This gives the energy-expression in Eq. 8, in which the symmetry of the SOEC's has been applied.

$$\rho_0 E(\boldsymbol{\eta}) = C_{11}\frac{\eta_1^2}{2} + C_{11}\frac{\eta_2^2}{2} + C_{33}\frac{\xi^2}{2} + C_{44}\frac{\eta_4^2}{2} + C_{44}\frac{\eta_5^2}{2} + \frac{1}{2}\left(C_{11} - C_{12}\right)\frac{\eta_6^2}{2} + C_{12}\eta_1\eta_2 + C_{13}\eta_1\xi + C_{13}\eta_2\xi \tag{8}$$

For large strains, the expansion in Eq. 8 is not sufficient and instead, TOEC's have to be included as well. The expansion of the strain energy up to the third order in strain is given in Eq. 9, in which the terms P are given in Eq. 10. Note that in Eq. 9, the symmetry of the SOEC's and TOEC's has been incorporated to simplify the resulting expression.

$$\begin{aligned}\rho_0 E(\boldsymbol{\eta}) = {} & C_{11}P_1 + C_{12}P_2 + C_{13}P_3 + C_{33}P_4 + C_{44}P_5 + C_{111}P_6 + C_{222}P_7 + C_{333}P_8 + \\ & C_{133}P_9 + C_{113}P_{10} + C_{112}P_{11} + C_{123}P_{12} + C_{144}P_{13} + C_{155}P_{14} + C_{344}P_{15}\end{aligned} \tag{9}$$

$$P_1 = \frac{\eta_1^2}{2} + \frac{\eta_2^2}{2} + \frac{\eta_6^2}{4}, \tag{10a}$$

$$P_2 = -\frac{\eta_6^2}{4} + \eta_1\eta_2, \tag{10b}$$

$$P_3 = \eta_1\xi + \eta_2\xi, \tag{10c}$$

$$P_4 = \frac{\xi^2}{2}, \tag{10d}$$

$$P_5 = \frac{\eta_4^2}{2} + \frac{\eta_5^2}{2}, \tag{10e}$$

$$P_6 = \frac{\eta_1^3}{6} + \frac{\eta_1\eta_2^2}{2} - \frac{\eta_1\eta_6^2}{4} + \frac{\eta_2\eta_6^2}{4}, \tag{10f}$$

$$P_7 = \frac{\eta_2^3}{6} - \frac{\eta_1\eta_2^2}{2} - \frac{\eta_2\eta_6^2}{8} + 3\frac{\eta_1\eta_6^2}{8}, \tag{10g}$$

$$P_8 = \frac{\xi^3}{6}, \tag{10h}$$

$$P_9 = \frac{\eta_1\xi^2}{2} + \frac{\eta_2\xi^2}{2}, \tag{10i}$$

$$P_{10} = \frac{\xi\eta_1^2}{2} + \frac{\xi\eta_2^2}{2} + \frac{\xi\eta_6^2}{4}, \tag{10j}$$

$$P_{11} = \frac{\eta_1^2\eta_2}{2} + \frac{\eta_1\eta_2^2}{2} - \frac{\eta_6^2\eta_1}{8} - \frac{\eta_6^2\eta_2}{8}, \tag{10k}$$

$$P_{12} = \eta_1\eta_2\xi - \frac{\xi\eta_6^2}{4}, \tag{10l}$$

$$P_{13} = \frac{\eta_1\eta_4^2}{2} + \frac{\eta_2\eta_5^2}{2} - \frac{\eta_4\eta_5\eta_6}{2}, \tag{10m}$$

$$P_{14} = \frac{\eta_2\eta_4^2}{2} + \frac{\eta_1\eta_5^2}{2} + \frac{\eta_4\eta_5\eta_6}{2}, \tag{10n}$$

$$P_{15} = \frac{\xi\eta_4^2}{2} + \frac{\xi\eta_5^2}{2} \tag{10o}$$

II. DETAILS OF CALCULATING TOEC'S

In this section, we consider again a deformation gradient $\mathbf{F}$, which leads to a Green-Lagrange strain, η, as defined in Eq. 11. As before, $\boldsymbol{\eta}$ has 6 independent components, indicated by $\eta_1, \eta_2, \eta_3, \eta_4, \eta_5, \eta_6$. In this section, expressions are derived relating the Lagrangian stress, Lagrangian strain, true stress, SOEC's and TOEC's for various crystal symmetries. Eq. 12 is the starting point for all these derivations. We also provide the form of the deformation gradients that give rise to desired Green-Lagrange strain tensors that are required for the calculation of specific (linear combinations) of SOEC's and TOEC's. The terms δ appearing in the deformation gradients represent distortions applied to the crystal. Note that the deformation gradients have to be carefully constructed as to leave only the desired (non-zero) elements in the resulting Green-Lagrange strain tensor.

$$\boldsymbol{\eta} = \frac{1}{2}\left(\boldsymbol{F}^T\boldsymbol{F} - \boldsymbol{I}\right) \tag{11}$$

$$t_{ij} = \rho_0 \frac{\partial E}{\eta_{ij}} \tag{12}$$

A. Cubic symmetry

$$\left.\begin{aligned} t_1\left(\eta_1\right) = \rho_0 \frac{\partial E}{\partial \eta_1}\Big|_{\eta_2=\eta_3=\eta_4=\eta_5=\eta_6=0} &= \frac{C_{111}\eta_1^2}{2} + C_{11}\eta_1 \\ \boldsymbol{F} &= \begin{bmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned}\right\} \tag{13}$$

$$\left.\begin{aligned} t_1\left(\eta_1\right) = \rho_0 \frac{\partial E}{\partial \eta_1}\Big|_{\eta_2=\eta_3=\eta_4=\eta_5=\eta_6=0} &= \frac{C_{112}\eta_1^2}{2} + C_{12}\eta_1 \\ \boldsymbol{F} &= \begin{bmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned}\right\} \tag{14}$$

$$\left.\begin{aligned} t_1\left(\eta_2,\eta_3\right) = \rho_0 \frac{\partial E}{\partial \eta_1}\Big|_{\substack{\eta_1=\eta_4=\eta_5=\eta_6=0 \\ \eta_2=\eta_3}} &= C_{12}\eta_3 + C_{12}\eta_2 + C_{123}\eta_2\eta_3 + C_{112}\frac{\eta_2^2}{2} + C_{112}\frac{\eta_3^2}{2} \\ \boldsymbol{F} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1+\delta & 0 \\ 0 & 0 & 1+\delta \end{bmatrix} \end{aligned}\right\} \tag{15}$$

$$\left.\begin{aligned} t_4\left(\eta_4\right) = \rho_0 \frac{\partial E}{\partial \eta_4}\Big|_{\eta_1=\eta_2=\eta_3=\eta_5=\eta_6=0} &= C_{44}\eta_4 \\ \boldsymbol{F} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & \sqrt{1-\delta^2} & \delta \\ 0 & \delta & \sqrt{1-\delta^2} \end{bmatrix} \end{aligned}\right\} \tag{16}$$

$$\left.\begin{aligned} t_4\left(\eta_1,\eta_4\right) = \rho_0 \frac{\partial E}{\partial \eta_4}\Big|_{\substack{\eta_2=\eta_3=\eta_5=\eta_6=0 \\ \eta_1=\eta_4}} &= C_{44}\eta_4 + C_{144}\eta_1\eta_4 \\ \boldsymbol{F} &= \begin{bmatrix} \frac{\delta}{2} + \sqrt{\delta\sqrt{1-\delta^2} - \frac{3\delta^2}{4} + 1} & 0 & 0 \\ 0 & \sqrt{1-\delta^2} & \delta \\ 0 & \delta & \sqrt{1-\delta^2} \end{bmatrix} \end{aligned}\right\} \tag{17}$$

$$\left.\begin{aligned} t_5\left(\eta_1,\eta_5\right) = \rho_0 \frac{\partial E}{\partial \eta_5}\Big|_{\substack{\eta_2=\eta_3=\eta_4=\eta_6=0 \\ \eta_1=\eta_5}} &= C_{44}\eta_5 + C_{155}\eta_1\eta_5 \\ \boldsymbol{F} &= \begin{bmatrix} \frac{\delta}{2} + \sqrt{\delta\sqrt{1-\delta^2} - \frac{3\delta^2}{4} + 1} & 0 & \delta \\ 0 & 1 & 0 \\ \delta & 0 & \sqrt{1-\delta^2} \end{bmatrix} \end{aligned}\right\} \tag{18}$$

$$\left.\begin{aligned} t_4\left(\eta_4,\eta_5,\eta_6\right) = \rho_0 \frac{\partial E}{\partial \eta_4}\Big|_{\substack{\eta_1=\eta_2=\eta_3=0 \\ \eta_4=\eta_5=\eta_6}} &= C_{44}\eta_4 + C_{456}\eta_5\eta_6 \\ \boldsymbol{F} &= \begin{bmatrix} \sqrt{1-\delta^2} & \delta & \delta \\ \delta & \sqrt{1-\delta^2} & \delta \\ \delta & \delta & \sqrt{1-\delta^2} \end{bmatrix} \end{aligned}\right\} \tag{19}$$

B. Hexagonal symmetry

$$\left.\begin{aligned} t_1(\eta_1) = \rho_0 \frac{\partial E}{\partial \eta_1}\Big|_{\eta_2=\eta_3=\eta_4=\eta_5=\eta_6=0} &= \frac{C_{111}\eta_1^2}{2} + C_{11}\eta_1 \\ \boldsymbol{F} &= \begin{bmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned}\right\} \tag{20}$$

$$\left.\begin{aligned} t_2(\eta_2) = \rho_0 \frac{\partial E}{\partial \eta_2}\Big|_{\eta_1=\eta_3=\eta_4=\eta_5=\eta_6=0} &= \frac{C_{222}\eta_2^2}{2} + C_{11}\eta_2 \\ \boldsymbol{F} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1+\delta & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned}\right\} \tag{21}$$

$$\left.\begin{aligned} t_3(\eta_3) = \rho_0 \frac{\partial E}{\partial \eta_3}\Big|_{\eta_1=\eta_2=\eta_4=\eta_5=\eta_6=0} &= \frac{C_{333}\eta_3^2}{2} + C_{33}\eta_3 \\ \boldsymbol{F} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+\delta \end{bmatrix} \end{aligned}\right\} \tag{22}$$

$$\left.\begin{aligned} t_3(\eta_1) = \rho_0 \frac{\partial E}{\partial \eta_3}\Big|_{\eta_2=\eta_3=\eta_4=\eta_5=\eta_6=0} &= \frac{C_{113}\eta_1^2}{2} + C_{13}\eta_1 \\ \boldsymbol{F} &= \begin{bmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned}\right\} \tag{23}$$

$$\left.\begin{aligned} t_1(\eta_3) = \rho_0 \frac{\partial E}{\partial \eta_1}\Big|_{\eta_1=\eta_2=\eta_4=\eta_5=\eta_6=0} &= \frac{C_{133}\eta_3^2}{2} + C_{13}\eta_3 \\ \boldsymbol{F} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1+\delta \end{bmatrix} \end{aligned}\right\} \tag{24}$$

$$\left.\begin{aligned} t_2(\eta_1) = \rho_0 \frac{\partial E}{\partial \eta_2}\Big|_{\eta_2=\eta_3=\eta_4=\eta_5=\eta_6=0} &= \frac{C_{112}\eta_1^2}{2} + C_{12}\eta_1 \\ \boldsymbol{F} &= \begin{bmatrix} 1+\delta & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned}\right\} \tag{25}$$

$$\left.\begin{aligned} t_4(\eta_4) = \rho_0 \frac{\partial E}{\partial \eta_4}\Big|_{\eta_1=\eta_2=\eta_3=\eta_5=\eta_6=0} &= C_{44}\eta_4 \\ \boldsymbol{F} &= \begin{bmatrix} 1 & 0 & 0 \\ 0 & \sqrt{1-\delta^2} & \delta \\ 0 & \delta & \sqrt{1-\delta^2} \end{bmatrix} \end{aligned}\right\} \tag{26}$$

$$\left.\begin{aligned} t_3(\eta_3,\eta_5) = \rho_0 \frac{\partial E}{\partial \eta_3}\Big|_{\substack{\eta_1=\eta_2=\eta_4=\eta_6=0 \\ \eta_3=\eta_5}} &= \frac{C_{333}\eta_3^2}{2} + C_{33}\eta_3 + \frac{C_{344}\eta_5^2}{2} \\ \boldsymbol{F} &= \begin{bmatrix} \sqrt{1-\delta^2} & 0 & \delta \\ 0 & 1 & 0 \\ \delta & 0 & \frac{\delta}{2} + \sqrt{\delta\sqrt{1-\delta^2} - \frac{3\delta^2}{4} + 1} \end{bmatrix} \end{aligned}\right\} \tag{27}$$

$$\left.\begin{aligned} t_5(\eta_3,\eta_5) = \rho_0 \frac{\partial E}{\partial \eta_5}\Big|_{\substack{\eta_1=\eta_2=\eta_4=\eta_6=0\\ \eta_3=\eta_5}} = C_{44}\eta_5 + C_{344}\eta_3\eta_5 \\ \boldsymbol{F} = \begin{bmatrix} \sqrt{1-\delta^2} & 0 & \delta \\ 0 & 1 & 0 \\ \delta & 0 & \frac{\delta}{2} + \sqrt{\delta\sqrt{1-\delta^2} - \frac{3\delta^2}{4} + 1} \end{bmatrix} \end{aligned}\right\} \tag{28}$$

$$\left.\begin{aligned} t_3(\eta_1,\eta_2) = \rho_0 \frac{\partial E}{\partial \eta_3}\Big|_{\substack{\eta_3=\eta_4=\eta_5=\eta_6=0\\ \eta_1=\eta_2}} = \frac{C_{113}\eta_1^2}{2} + C_{123}\eta_1\eta_2 + C_{13}\eta_1 + \frac{C_{113}\eta_2^2}{2} + C_{13}\eta_2 \\ \boldsymbol{F} = \begin{bmatrix} 1+\delta & 0 & 0 \\ 0 & 1+\delta & 0 \\ 0 & 0 & 1 \end{bmatrix} \end{aligned}\right\} \tag{29}$$

$$\left.\begin{aligned} t_4(\eta_1,\eta_4) = \rho_0 \frac{\partial E}{\partial \eta_4}\Big|_{\substack{\eta_2=\eta_3=\eta_5=\eta_6=0\\ \eta_1=\eta_4}} = C_{44}\eta_4 + C_{144}\eta_1\eta_4 \\ \boldsymbol{F} = \begin{bmatrix} \frac{\delta}{2} + \sqrt{\delta\sqrt{1-\delta^2} - \frac{3\delta^2}{4} + 1} & 0 & 0 \\ 0 & \sqrt{1-\delta^2} & \delta \\ 0 & \delta & \sqrt{1-\delta^2} \end{bmatrix} \end{aligned}\right\} \tag{30}$$

$$\left.\begin{aligned} t_5(\eta_1,\eta_5) = \rho_0 \frac{\partial E}{\partial \eta_5}\Big|_{\substack{\eta_2=\eta_3=\eta_4=\eta_6=0\\ \eta_1=\eta_5}} = C_{44}\eta_5 + C_{155}\eta_1\eta_5 \\ \boldsymbol{F} = \begin{bmatrix} \frac{\delta}{2} + \sqrt{\delta\sqrt{1-\delta^2} - \frac{3\delta^2}{4} + 1} & 0 & \delta \\ 0 & 1 & 0 \\ \delta & 0 & \sqrt{1-\delta^2} \end{bmatrix} \end{aligned}\right\} \tag{31}$$