ElastoPlasticQPot – An implementation for an elasto-plastic continuum model based on a manifold of quadratic potentials

T.W.J. de Geus

*Contact: tom@geus.me – www.geus.me – https://github.com/tdegeus/ElastoPlasticQPot

Abstract

A microscopic continuum model of plasticity in amorphous solids is proposed. This model uses a strain energy with multiple minima to capture the effect of plasticity. This model is derived from the work of Jagla (2017).

Keywords: elasto-plasticity; linear elasticity

Contents

1 General model

1.1 Constitutive model

The model is constructed such that it behaves linear elastically in the volumetric stress response. The same holds for the deviatoric stress response, whereby plasticity is modelled such that the material starts flowing once a critical strain is reached. After a period of flow, the deviatoric stress response is again linear elastic. A detail to mention upfront is that the elastic moduli and the equivalent stress and strain are defined such that the model is equivalent regardless of the number of dimensions, d, and the shear modulus is defined as $\sigma_{xy} = G \varepsilon_{xy}$ (which is common in elastodynamics). To retrieve another common definition for linear elasticity in $d = 3$, one simply has to rescale the parameters. See Section 1.2 for the nomenclature, including the parameter transformation.

The model is based on a strain energy W that is composed of two parts, a volumetric (or hydrostatic) part U related to the hydrostatic strain ε_{m}, and a shear (or deviatoric) part V related to the equivalent shear strain ε_{d}, i.e.

$$W(\underline{\varepsilon}) = U(\varepsilon_{m}) + V(\varepsilon_{d}) \tag{1}$$

The stress response $\underline{\sigma}$ is the derivative of this energy with respect to the strain tensor $\underline{\varepsilon}$. Before specialising U and V we can already say that

$$\underline{\sigma} = \frac{\partial W}{\partial \underline{\varepsilon}} = \frac{\partial U}{\partial \varepsilon_{m}} \frac{\partial \varepsilon_{m}}{\partial \underline{\varepsilon}} + \frac{\partial V}{\partial \varepsilon_{d}} \frac{\partial \varepsilon_{d}}{\partial \underline{\varepsilon}} = \frac{\partial U}{\partial \varepsilon_{m}} \frac{1}{d} \underline{I} + \frac{\partial V}{\partial \varepsilon_{d}} \frac{\underline{\varepsilon}_{d}}{2 \, \varepsilon_{d}} \tag{2}$$

From which we can identity the hydrostatic stress and the deviatoric stress tensor as

$$\sigma_{m} = \frac{1}{d} \frac{\partial U}{\partial \varepsilon_{m}} \, , \qquad \underline{\sigma}_{d} = \frac{\partial V}{\partial \varepsilon_{d}} \frac{\underline{\varepsilon}_{d}}{2 \, \varepsilon_{d}} \tag{3}$$

Below, both $U(\varepsilon_{m})$ and $V(\varepsilon_{d})$ will be defined by slowly increase complexity, departing from linear elasticity.

1.1.1 Linear elasticity

We start simple by considering linear elasticity. In this case the volumetric strain energy U and the shear strain energy V read

$$U(\varepsilon_{m}) = \frac{d}{2} K \varepsilon_{m}^{2} \, , \qquad V(\varepsilon_{d}) = G \varepsilon_{d}^{2} \tag{4}$$

The two potentials are plotted in Fig. 1 (in which only $\varepsilon_{d} \geq 0$ is shown, as it is by definition non-negative). It is trivial to obtain that

$$\frac{\partial U}{\partial \varepsilon_{m}} = d K \varepsilon_{m} \, , \qquad \frac{\partial V}{\partial \varepsilon_{d}} = 2 G \varepsilon_{d} \tag{5}$$

(plotted in Fig. 2). From which we obtain the following expression for the stress

$$\underline{\sigma}(\underline{\varepsilon}) = K \varepsilon_{m} \underline{I} + G \underline{\varepsilon}_{d} \tag{6}$$

1.1.2 Plastic potential – Parabolic potential with multiple minima

The model is now extended to account for plasticity. The model is defined such that the material responds volumetrically purely elastic, while in shear the model is governed by multiple minima. These minima have the effect that when the material reaches a certain yield stress, it jumps to the next minimum. Around this minimum the elasticity is always the same. When loading is continued the the material again jumps to a new minimum when the next yield stress is reached. The magnitude of the jumps and of the yield stress are thereby related.

As described, the volumetric behaviour is simply elastic; whereby the potential is given by Eq. (4a) and is plotted in Fig. 1(a). To attain the desired behaviour in shear, the equivalent shear strain space is divided in a finite number of yield strains $\varepsilon_{y}^{(0)}, \varepsilon_{y}^{(1)}, \varepsilon_{y}^{(2)}, \dots$. A parabolic potential is then defined between each pair ($[\varepsilon_{y}^{(0)}, \varepsilon_{y}^{(1)}$), $[\varepsilon_{y}^{(1)}, \varepsilon_{y}^{(2)}$), ...).

The shear strain energy is then composed of a manifold of quadratic contributions

$$V\left(\varepsilon_{y}^{(i)} \leq \varepsilon_{d} < \varepsilon_{y}^{(i+1)}\right) = V^{(i)} = G \left[\left[\varepsilon_{d} - \varepsilon_{min}^{(i)} \right]^{2} - \left[\Delta \varepsilon_{y}^{(i)} \right]^{2} \right] \tag{7}$$
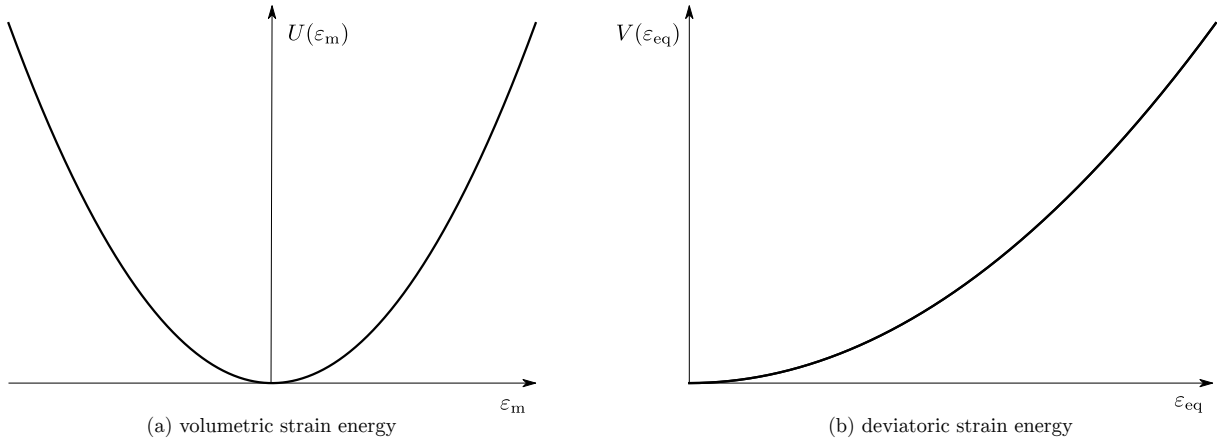
(a) volumetric strain energy   (b) deviatoric strain energy

Figure 1. Strain energy $W(\underline{\varepsilon}) = U(\varepsilon_\mathrm{m}) + V(\varepsilon_\mathrm{d})$ for linear elasticity.

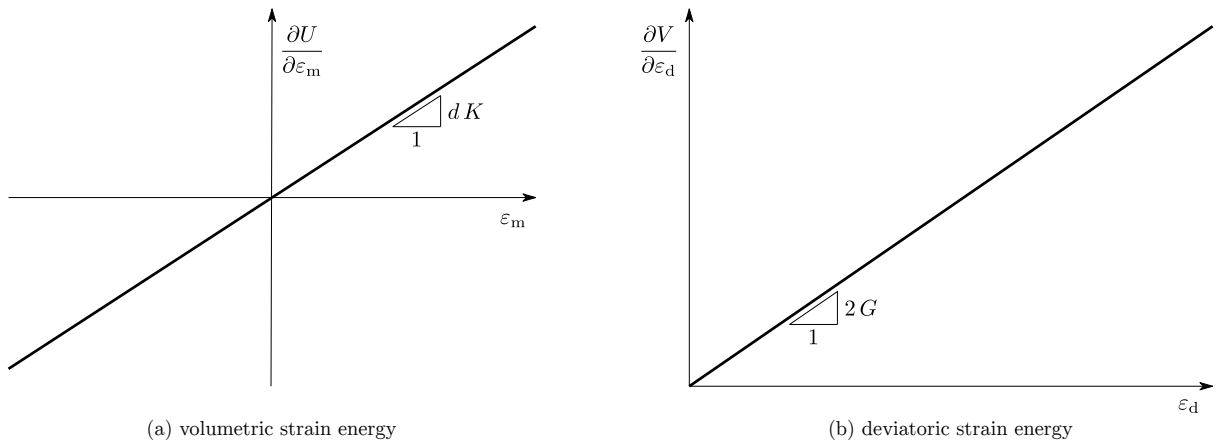(a) volumetric strain energy   (b) deviatoric strain energy

Figure 2. Derivative of the hydrostatic strain energy U and the deviatoric strain energy V w.r.t. respectively the hydrostatic strain ε_m and the equivalent shear strain ε_d.

where the mean of $\varepsilon_y^{(i)}$ and $\varepsilon_y^{(i+1)}$ is

$$\varepsilon_{\min}^{(i)} = \frac{1}{2}\left[\varepsilon_y^{(i+1)} + \varepsilon_y^{(i)}\right] \tag{8}$$

which is also the equivalent shear strain at which the shear strain energy reaches its minimum. From this minimum, the distance to $\varepsilon_y^{(i)}$ and $\varepsilon_y^{(i+1)}$ is

$$\Delta\varepsilon_y^{(i)} = \frac{1}{2}\left[\varepsilon_y^{(i+1)} - \varepsilon_y^{(i)}\right] \tag{9}$$

The resulting shear strain energy is plotted in Fig. 3(a).

The stress response is obtained from

$$\frac{\partial V^{(i)}}{\partial \varepsilon_d} = 2\,G\left[\varepsilon_d - \varepsilon_{\min}^{(i)}\right] \tag{10}$$

(see Fig. 4(a)). From which it can be observed that in elasticity the behaviour is identical to above (cf. (2b)). For the case that $\varepsilon_y^{(0)} = -\varepsilon_y^{(1)}$ the responses are even identical until initial yield stress is reached. For completeness, the stress reads

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}) = K\,\varepsilon_m\,\boldsymbol{I} + G\left[1 - \varepsilon_{\min}^{(i)}/\varepsilon_d\right]\boldsymbol{\varepsilon}_d \qquad \text{for } \varepsilon_y^{(i)} \leq \varepsilon_d < \varepsilon_y^{(i+1)} \tag{11}$$

whereby one has to assume that when $\varepsilon_d = 0$ also $\boldsymbol{\sigma}_d = \underline{0}$ in order to avoid zero division. The response is plotted in Fig. 4(a), from which it is observed that it exhibits stress jumps between different parabola in the potential, because of the discontinuity in the second derivative of the elastic potential. This can be remedied, such as in the model presented below.

1.1.3   Plastic potential – Smooth parabolic potential with multiple minima

The remedy the discontinuity in the second derivative of the potential, it is smoothened as follows:

$$V\!\left(\varepsilon_y^{(i)} \leq \varepsilon_d < \varepsilon_y^{(i+1)}\right) = V^{(i)} = -2\,G\left[\frac{\Delta\varepsilon_y^{(i)}}{\pi}\right]^2\left[1 + \cos\left(\frac{\pi}{\Delta\varepsilon_y^{(i)}}\left[\varepsilon_d - \varepsilon_{\min}^{(i)}\right]\right)\right] \tag{12}$$

which is plotted in Fig. 3(b). In this case the stress is obtained from

$$\frac{\partial V^{(i)}}{\partial \varepsilon_d} = 2\,G\left[\frac{\Delta\varepsilon_y^{(i)}}{\pi}\right]\sin\left(\frac{\pi}{\Delta\varepsilon_y^{(i)}}\left[\varepsilon_d - \varepsilon_{\min}^{(i)}\right]\right) \tag{13}$$

(see Fig. 4(b)). Which is to the first order equal to linear elasticity around its minimum $\varepsilon_{\min}^{(i)}$. Indeed, the first order Taylor series of Eq. (13) around $\varepsilon_d = \varepsilon_{\min}^{(i)}$,

$$\frac{\partial V^{(i)}}{\partial \varepsilon_d} \approx 2\,G\left[\varepsilon_d - \varepsilon_{\min}^{(i)}\right] \tag{14}$$

is identical to Eq. (10).

For completeness, also in case the expression for the entire stress tensor

$$\boldsymbol{\sigma}(\boldsymbol{\varepsilon}) = K\,\varepsilon_m\,\boldsymbol{I} + G\left[\frac{\Delta\varepsilon_y^{(i)}}{\pi}\right]\sin\left(\frac{\pi}{\Delta\varepsilon_y^{(i)}}\left[\varepsilon_d - \varepsilon_{\min}^{(i)}\right]\right)\frac{\boldsymbol{\varepsilon}_d}{\varepsilon_d} \qquad \text{for } \varepsilon_y^{(i)} \leq \varepsilon_d < \varepsilon_y^{(i+1)} \tag{15}$$

whereby, again, one has to assume that when $\varepsilon_d = 0$ also $\boldsymbol{\sigma}_d = \underline{0}$ in order to avoid zero division.

(a) multi-parabolic potential

(b) smooth multi-parabolic potential
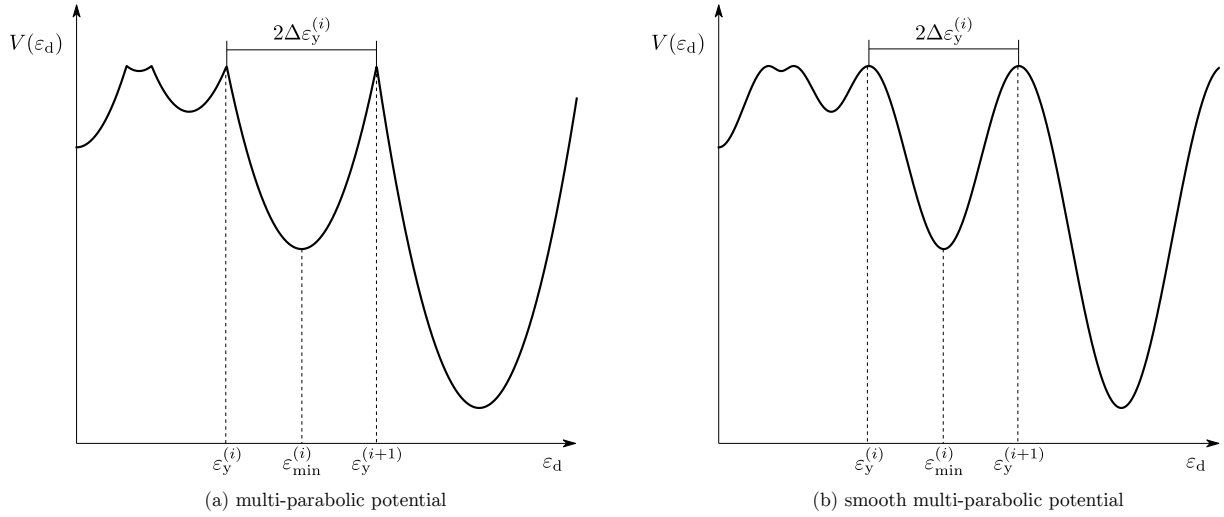
Figure 3. The multi-minima shear strain energy, $V(\varepsilon_\mathrm{d})$, that models the effect of plasticity. The multi-parabolic shear strain energy is shown in (a), while its smoothened equivalent is shown in (b).
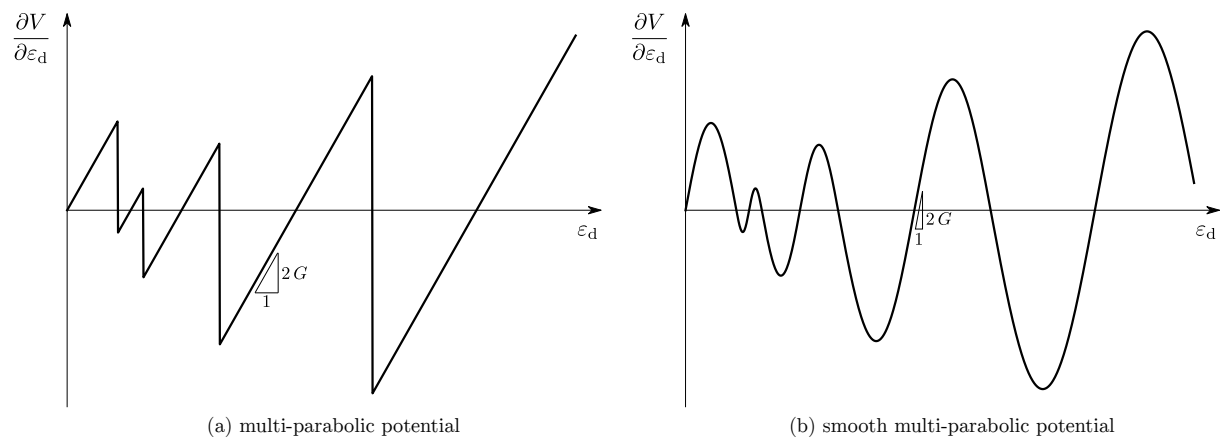

(a) multi-parabolic potential

(b) smooth multi-parabolic potential

Figure 4. Derivative of the shear strain energy V.

1.2   Nomenclature

1.2.1   Tensors and tensor products

- Second order tensor

$$\underline{A} = A_{ij}\vec{e}_i\vec{e}_j \tag{16}$$

- Dyadic tensor product

$$\underline{C} = \vec{a} \otimes \vec{b} \tag{17}$$
$$C_{ij} = a_i\,b_j \tag{18}$$

- Double tensor contraction

$$C = \underline{A} : \underline{B} = \mathrm{tr}\left(\underline{A} \cdot \underline{B}\right) \tag{19}$$
$$= A_{ij}\,B_{ji} \tag{20}$$

- Deviatoric projection tensor (in d dimensions)

$$\mathbb{I}_{\mathrm{d}} = \mathbb{I}_{\mathrm{s}} - \tfrac{1}{d}\underline{I} \otimes \underline{I} \tag{21}$$

1.2.2   Strain measures

- Mean strain (in d dimensions)

$$\varepsilon_{\mathrm{m}} = \tfrac{1}{d}\,\mathrm{tr}(\underline{\varepsilon}) = \tfrac{1}{d}\,\underline{\varepsilon} : \underline{I} \tag{22}$$

- Strain deviator

$$\underline{\varepsilon}_{\mathrm{d}} = \underline{\varepsilon} - \varepsilon_{\mathrm{m}}\,\underline{I} = \mathbb{I}_{\mathrm{d}} : \underline{\varepsilon} \tag{23}$$

- Equivalent shear strain

$$\varepsilon_{\mathrm{d}} = \sqrt{\tfrac{1}{2}\,\underline{\varepsilon}_{\mathrm{d}} : \underline{\varepsilon}_{\mathrm{d}}} \tag{24}$$

- Equivalent strain

$$\varepsilon_{\mathrm{eq}} = \sqrt{\tfrac{1}{2}\,\underline{\varepsilon} : \underline{\varepsilon}} \tag{25}$$

1.2.3   Stress measures

- Mean stress (in d dimensions)

$$\sigma_{\mathrm{m}} = \tfrac{1}{d}\,\mathrm{tr}(\underline{\sigma}) = \tfrac{1}{d}\,\underline{\sigma} : \underline{I} \tag{26}$$

- Stress deviator

$$\underline{\sigma}_{\mathrm{d}} = \underline{\sigma} - \sigma_{\mathrm{m}}\,\underline{I} = \mathbb{I}_{\mathrm{d}} : \underline{\sigma} \tag{27}$$

- Von Mises equivalent shear stress

$$\sigma_{\mathrm{d}} = \sqrt{\tfrac{1}{2}\,\underline{\sigma}_{\mathrm{d}} : \underline{\sigma}_{\mathrm{d}}} \tag{28}$$

- Equivalent stress

$$\sigma_{\mathrm{eq}} = \sqrt{\tfrac{1}{2}\,\underline{\sigma} : \underline{\sigma}} \tag{29}$$

1.2.4 Derivatives

- Strain deviator

$$\frac{\partial \underline{\varepsilon}_{\mathrm{d}}}{\partial \underline{\varepsilon}} = \mathbb{I}_{\mathrm{d}} \tag{30}$$

- Mean equivalent shear strain (in d dimensions)

$$\frac{\partial \varepsilon_{\mathrm{m}}}{\partial \underline{\varepsilon}} = \tfrac{1}{d}\underline{\boldsymbol{I}} : \mathbb{I} = \tfrac{1}{d}\underline{\boldsymbol{I}} \tag{31}$$

- Equivalent shear strain

$$\frac{\partial \varepsilon_{\mathrm{d}}}{\partial \underline{\varepsilon}} = \frac{1}{2\,\varepsilon_{\mathrm{d}}}\frac{1}{2}\big[\,\mathbb{I}_{\mathrm{d}} : \underline{\varepsilon}_{\mathrm{d}} + \underline{\varepsilon}_{\mathrm{d}} : \mathbb{I}_{\mathrm{d}}\,\big] = \frac{\underline{\varepsilon}_{\mathrm{d}}}{2\,\varepsilon_{\mathrm{d}}} \tag{32}$$

1.2.5 Conversion to common parameters for linear elasticity

The parameters are confronted to their common definitions (denoted here with a tilde) for linear elasticity in $d = 3$:

- Hydrostatic strain

$$\tilde{\varepsilon}_{\mathrm{m}} = \varepsilon_{\mathrm{m}} \tag{33}$$

- Equivalent shear strain

$$\tilde{\varepsilon}_{\mathrm{eq}} = \sqrt{\tfrac{2}{3}\underline{\varepsilon}_{\mathrm{d}} : \underline{\varepsilon}_{\mathrm{d}}} = \sqrt{\tfrac{4}{3}}\,\varepsilon_{\mathrm{d}} \tag{34}$$

- Hydrostatic stress

$$\tilde{\sigma}_{\mathrm{m}} = \sigma_{\mathrm{m}} \tag{35}$$

- Von Mises equivalent shear stress

$$\tilde{\sigma}_{\mathrm{eq}} = \sqrt{\tfrac{3}{2}\underline{\boldsymbol{\sigma}}_{\mathrm{d}} : \underline{\boldsymbol{\sigma}}_{\mathrm{d}}} = \sqrt{3}\,\sigma_{\mathrm{eq}} \tag{36}$$

- Bulk modulus

$$\tilde{K} = 3\,K \tag{37}$$

- Shear modulus

$$\tilde{G} = G/2 \tag{38}$$

This results in a stress response

$$\underline{\boldsymbol{\sigma}}(\underline{\varepsilon}) = 3\tilde{K}\,\varepsilon_{\mathrm{m}}\,\underline{\boldsymbol{I}} + 2\tilde{G}\,\underline{\varepsilon}_{\mathrm{d}} \tag{39}$$

or, in slightly different notation

$$\underline{\boldsymbol{\sigma}}(\underline{\varepsilon}) = \tilde{K}\,\mathrm{tr}\,(\varepsilon_{\mathrm{m}})\,\underline{\boldsymbol{I}} + 2\tilde{G}\,\big[\underline{\varepsilon} - \tfrac{1}{3}\mathrm{tr}\,(\varepsilon_{\mathrm{m}})\,\underline{\boldsymbol{I}}\big] \tag{40}$$

Note that the equivalent stress and strain are defined such that they are work conjugate (i.e. $\tilde{\sigma}_{\mathrm{eq}}\,\tilde{\varepsilon}_{\mathrm{eq}} = \underline{\boldsymbol{\sigma}} : \underline{\varepsilon}$) for uniaxial extension of an incompressible material.

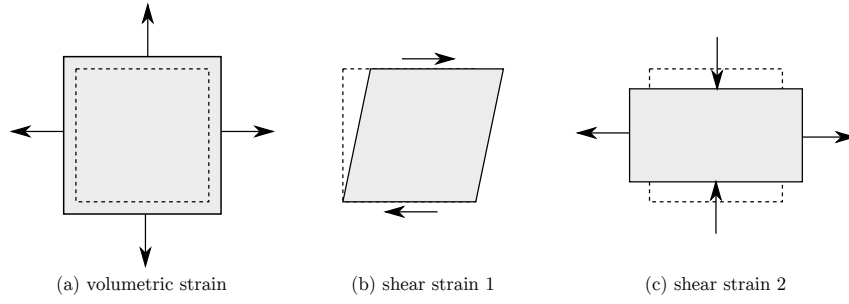(a) volumetric strain   (b) shear strain 1   (c) shear strain 2

Figure 5. The three independent modes described by a 2-d stain tensor $\underline{\varepsilon}$.

2   Specialized model – planar shear

2.1   Motivation

The model as proposed above treats all shear modes equally (because V is function of ε_{d}). Consequently it is isotropic. There are, however, cases for which an anisotropic model is more realistic. Below a model is proposed in which the plasticity can only occur along a specific plane. Before that, the claim of isotropy is further motivated in two dimensions. In that case the strain tensor has three independent modes, illustrated in Fig. 5.

The first shear mode, in Fig. 5(b), corresponds to a strain tensor of the following structure

$$\underline{\underline{\varepsilon}} = \begin{bmatrix} 0 & \gamma \\ \gamma & 0 \end{bmatrix} \tag{41}$$

The second shear mode, in Figure 5(c), corresponds to the same shear deformation rotated by $-\pi/4$. It is therefore of the structure

$$\underline{\underline{\varepsilon}} = \begin{bmatrix} \gamma & 0 \\ 0 & -\gamma \end{bmatrix} \tag{42}$$

In terms of the equivalent shear strain, both modes result in $\varepsilon_{\mathrm{d}} = |\gamma|$. This is further illustrated by rotating the strain tensor from Eq. (41) by an angle θ:

$$\underline{\underline{\varepsilon}}' = \underline{\underline{R}}\,\underline{\underline{\varepsilon}}\,\underline{\underline{R}}^T \tag{43}$$

where the rotation matrix depends on the rotation angle θ as follows

$$\underline{\underline{R}} = \begin{bmatrix} \cos\theta & -\sin\theta \\ \sin\theta & \cos\theta \end{bmatrix} \tag{44}$$

Trivially $\varepsilon_{\mathrm{d}} = |\gamma|$, independent of θ – as plotted in Fig 6 in black. The contributions of the two shear modes are examined by examining ε'_{xy}, representative of the first shear mode in Fig. 5(b), and ε'_{xx}, representative of the second shear mode in Fig. 5(c). These contributions are plotted in Fig. 6 respectively in green and red. Indeed, the contributions of the two shear modes vary with θ, while ε_{d} it is oblivious to this rotation.

2.2   Model

In this model, the plasticity will be localised on a plane with normal $\vec{n}$ (which has unit length $||\vec{n}|| \equiv 1$), see Fig. 7. To do so, the strain deviator $\underline{\varepsilon}_{\mathrm{d}}$ is decomposed in two parts, the strain along the plastic ('weak') plane $\underline{\varepsilon}_{\mathrm{s}}$, and the remaining strain $\underline{\varepsilon}_{\mathrm{n}}$. I.e.

$$\underline{\varepsilon}_{\mathrm{d}} = \underline{\varepsilon}_{\mathrm{s}} + \underline{\varepsilon}_{\mathrm{n}} \tag{45}$$

To compute the former, planar strain tensor $\underline{\varepsilon}_{\mathrm{s}}$, first the direction of the deviatoric stain tensor projected on the plane is determined as

$$\vec{s}_{\mathrm{n}} = \frac{\underline{\varepsilon}_{\mathrm{d}} \cdot \vec{n}}{||\,\underline{\varepsilon}_{\mathrm{d}} \cdot \vec{n}\,||} \tag{46}$$
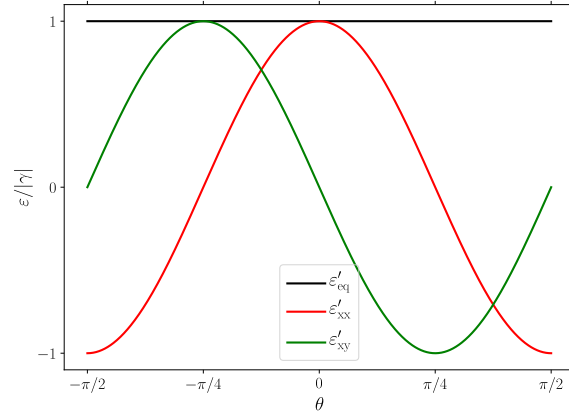
Figure 6. Comparison between the equivalent shear strain $2\varepsilon_\mathrm{d}^2 = \underline{\varepsilon}_\mathrm{d} : \underline{\varepsilon}_\mathrm{d}$ the strain along the x-plane, $\varepsilon_\mathrm{ss} = \vec{e}_x \cdot \underline{\varepsilon} \cdot \vec{e}_y$, and the strain perpendicular to it, $\varepsilon_\mathrm{ps} = \vec{e}_x \cdot \underline{\varepsilon} \cdot \vec{e}_x$.

The strain direction along the plane is now found by projecting $\vec{s}_\mathrm{n}$ on it:

$$\vec{s} = \frac{\vec{s}_\mathrm{n} - (\vec{s}_\mathrm{n} \cdot \vec{n}) \, \vec{n}}{|| \, \vec{s}_\mathrm{n} - (\vec{s}_\mathrm{n} \cdot \vec{n}) \, \vec{n} \, ||} \tag{47}$$

The amount of strain in this direction is finally found to be

$$\varepsilon_\mathrm{s} = \vec{s} \cdot \underline{\varepsilon}_\mathrm{d} \cdot \vec{n} \tag{48}$$

Not that ε_s is by definition non-negative, i.e. it is oblivious to rotations about $\vec{n}$.

The planar deviatoric strain tensor can now be constructed:

$$\underline{\varepsilon}_\mathrm{s} = \varepsilon_\mathrm{s} \left(\vec{s} \otimes \vec{n} + \vec{n} \otimes \vec{s} \right) \tag{49}$$

From this it is obvious that ε_s is the equivalent shear strain of this tensor, i.e.

$$\varepsilon_\mathrm{s} \equiv \sqrt{\tfrac{1}{2} \underline{\varepsilon}_\mathrm{s} : \underline{\varepsilon}_\mathrm{s}} \tag{50}$$

(To show this one has to use that $\vec{n} \cdot \vec{n} \equiv 1$ and $\vec{s} \cdot \vec{s} \equiv 1$ while $\vec{n} \cdot \vec{s} \equiv 0$).
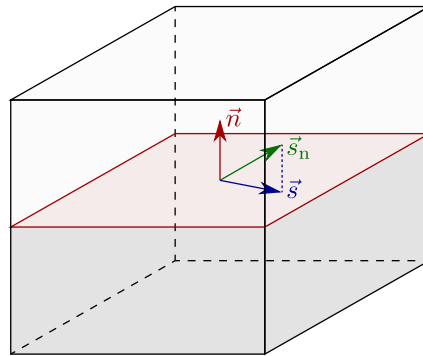

Figure 7. Strain along a plane defined by its normal $\vec{n}$: the strain vector $\vec{s}_\mathrm{n}$ and its planar projection $\vec{s}$.

The remaining strain can now be trivially obtained from Eq. (45) as

$$\underline{\varepsilon}_\mathrm{n} = \underline{\varepsilon}_\mathrm{d} - \underline{\varepsilon}_\mathrm{s} \tag{51}$$

Its equivalent shear strain reads

$$\varepsilon_\mathrm{n} = \sqrt{\tfrac{1}{2} \underline{\varepsilon}_\mathrm{n} : \underline{\varepsilon}_\mathrm{n}} \tag{52}$$

For plasticity to occur only along the 'weak' plane, the shear strain energy is further decomposed in a planar part V_s that will be plastic, and a non-planar part V_n that will be elastic:

$$V = V_\mathrm{s}(\varepsilon_\mathrm{s}) + V_\mathrm{n}(\varepsilon_\mathrm{n}) \tag{53}$$

Based on the definitions of the elastic and plastic potentials the following expression for the stress is obtained

$$\underline{\boldsymbol{\sigma}}(\underline{\boldsymbol{\varepsilon}}) = K\,\varepsilon_\mathrm{m}\,\underline{\boldsymbol{I}} + G\,\underline{\boldsymbol{\varepsilon}}_\mathrm{n} + G\left[\frac{\Delta\varepsilon_\mathrm{y}^{(i)}}{\pi}\right]\sin\left(\frac{\pi}{\Delta\varepsilon_\mathrm{y}^{(i)}}\left[\varepsilon_\mathrm{s} - \varepsilon_\mathrm{min}^{(i)}\right]\right)\frac{\underline{\boldsymbol{\varepsilon}}_\mathrm{s}}{\varepsilon_\mathrm{s}} \quad \text{for } \varepsilon_\mathrm{y}^{(i)} \leq \varepsilon_\mathrm{s} < \varepsilon_\mathrm{y}^{(i+1)} \tag{54}$$

References

Jagla, E. (2017). Different universality classes at the yielding transition of amorphous systems. *Phys. Rev. E*, 96(2):023006.