The neutron star crust

Elasticity, breaking strength, durability and enhancement of the thermonuclear reaction rates

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Introduction: personal history

An optional course on the "Fusion power" at school (1997-1998 yrs?):

One of the questions in a test:

- Which interactions are crucial for the neutron stars?

My answer:

- Nuclear, gravitational and (after some thinking) electromagnetic

Teacher:

- It's not true. Electromagnetic interactions are not important, because neutron stars consist of neutral neutrons.

This talk is about the role of the electrostatic interactions in the neutron star crust

Part I: crust as a solid body

Some key questions

[from INT workshop INT-18-71W, Astro-Solids, Dense Matter, and Gravitational Waves, April 16-20, 2018]

- What is the minimum, typical, and maximum ellipticity one should expect?

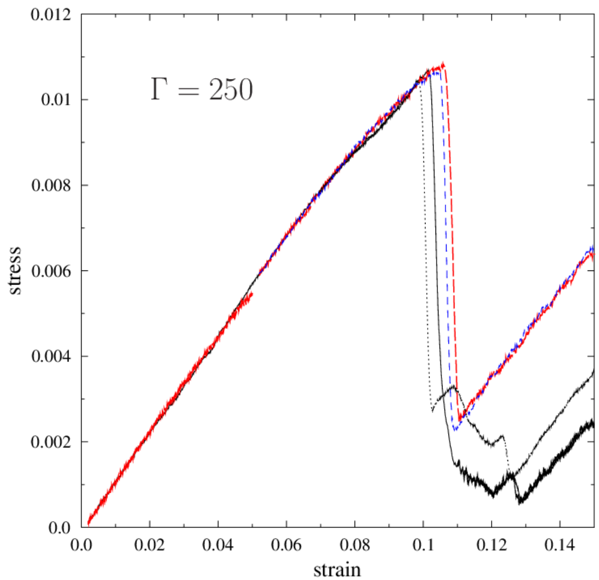
What is the strength (breaking strain) of the crust?

- How does strain evolve in the crust and how does it break?

- What are the implications of observed upper limits on the ellipticity?

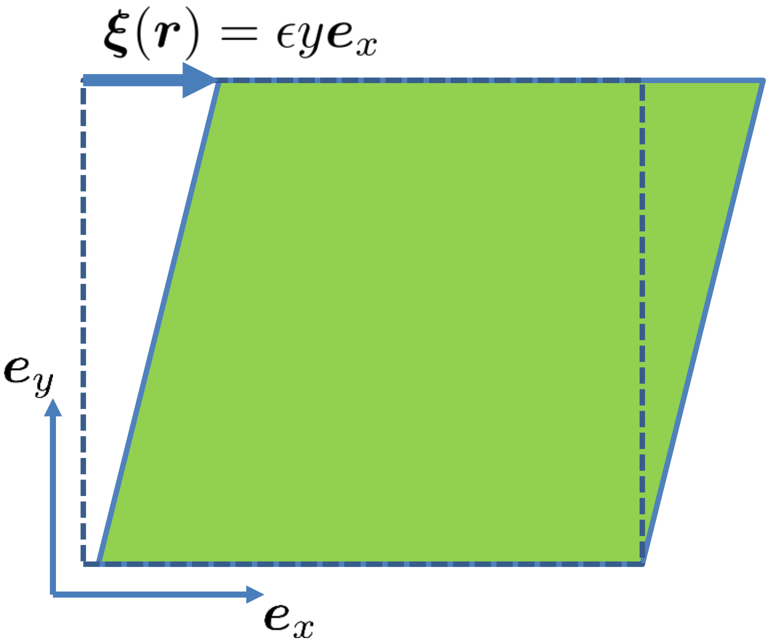
- At what point do upper limits become “interesting” (e.g. constrain theory)?

- What are possible mountain building mechanisms (such as asymmetric accretion, temperature gradients, magnetic stress...)?



Typical stress-strain curves
[MD simulations]

Introduction: Theory of Elasticity



Deformation: $\boldsymbol{r} \to \boldsymbol{r} + \boldsymbol{\xi}(\boldsymbol{r})$

Displacement gradient $u_{ij} = \dfrac{\partial \xi_i}{\partial x_j}$

Lagrangian strain parameters

$$\eta_{ij} = \eta_{ji} = \frac{1}{2}\left(u_{ij} + u_{ji} + u_{li}u_{lj}\right)$$

Forces

(to volume element from nearby elements)

$$f_i = \frac{\partial \sigma_{ij}}{\partial x_j}$$

In the crust

$$\sigma_{ij} = -P\delta_{ij} + \delta\sigma_{ij}$$

EOS

(electrons+neutrons+undeformed lattice)

Elastic part

$\delta\sigma_{ij}(u_{ij})$

Elastic part of stress tensor

Microphysics: $$\delta\sigma_{ij} = \delta\sigma_{ij}(u_{ij}, \dots)$$

$$\boxed{\delta\sigma_{ij} \lesssim 10^{-3} P_e}$$

$\underline{\text{Reminder:}}$ Traditional case $P = 0$

$$\delta^{(2)}\mathcal{E} = \frac{1}{2} C_{ijkl}\eta_{ij}\eta_{kl} = \frac{1}{2} S_{ijkl} u_{ij} u_{kl}$$

$$\mathcal{E} = \rho_0 \, E$$

Density at not deformed state, i.e. corresponding to $\boldsymbol{\xi} = 0 \;\; \Rightarrow \eta_{ij} = u_{ij} = 0$

Energy per unit mass at given deformation

$\boxed{\text{Generally, } \mathcal{E} \text{ is not equal to the energy density}}$

Elastic part of stress tensor

Microphysics: $$\delta\sigma_{ij} = \delta\sigma_{ij}(u_{ij}, \ldots)$$

$$\boxed{\delta\sigma_{ij} \lesssim 10^{-3} P_e}$$

Reminder: Traditional case $P = 0$

$$\delta^{(2)}\mathcal{E} = \frac{1}{2} C_{ijkl}\eta_{ij}\eta_{kl} = \frac{1}{2} S_{ijkl} u_{ij} u_{kl}$$

$$\sigma_{ij} = \frac{1}{2} B_{ijkl}\left(u_{kl} + u_{lk}\right)$$

$$P = 0 \Rightarrow \quad \boxed{C_{ijkl} = S_{ijkl} = B_{ijkl}}$$

Voigt symmetry: $C_{ijkl} = C_{jikl} = C_{klij}$ - up to 21 coefficients

Elastic part of stress tensor

Microphysics: $$\delta\sigma_{ij} = \delta\sigma_{ij}(u_{ij}, \ldots)$$

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$$\sigma_{ij} = \frac{1}{2} B_{ijkl}\left(u_{kl} + u_{lk}\right)$$

For cubic crystal 3 independent coefficients:

$$c_{11} = C_{xxxx}, \quad c_{12} = C_{xxyy}, \quad c_{44} = C_{xyxy}$$

Isotropic material: $$\delta^{(2)}\mathcal{E} = \mu\left(u_{ik} - \tfrac{1}{3}\delta_{ik} u_{ll}\right)^2 + \tfrac{K}{2} u_{ll}^2$$

Elastic part of stress tensor

Microphysics: $$\delta\sigma_{ij} = \delta\sigma_{ij}(u_{ij}, \ldots)$$

$$\boxed{\delta\sigma_{ij} \lesssim 10^{-3} P_e}$$

Neutron star crust: $P \neq 0$ [Wallace (1967), Baiko (2011), see also Marcus & Qiu (2009)]

$$\delta\mathcal{E} = \boxed{-P\delta_{ij}\eta_{ij}} + \frac{1}{2}C_{ijkl}\eta_{ij}\eta_{kl} = -P\delta_{ij}u_{ij} + \frac{1}{2}S_{ijkl}u_{ij}u_{kl}$$

$$\delta\sigma_{ij} = \frac{1}{2}B_{ijkl}\left(u_{kl} + u_{lk}\right)$$

$$P \neq 0 \Rightarrow \quad \boxed{C_{iklm} \neq S_{iklm} \neq B_{iklm}}$$

Voigt symmetry: $C_{ijkl} = C_{jikl} = C_{klij}$ - up to 21 coefficients

$$B_{ijkl} = B_{jikl} = B_{klij}$$

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$$\delta\sigma_{ij} = \frac{1}{2}B_{ijkl}\left(u_{kl} + u_{lk}\right)$$

$$P \neq 0 \Rightarrow \quad \boxed{C_{iklm} \neq S_{iklm} \neq B_{iklm}}$$

Why the theory becomes so complicated and should we care for it?

Elasticity under finite pressure

[Wallace (1967), Baiko (2011), see also Marcus & Qiu (2009)]

$$\delta\mathcal{E} = \boxed{-P\delta_{ij}\eta_{ij}} + \frac{1}{2}C_{ijkl}\eta_{ij}\eta_{kl} = -P\delta_{ij}u_{ij} + \frac{1}{2}S_{ijkl}u_{ij}u_{kl}$$

Associated with $\delta E = -P\delta V$

$$P \neq 0 \Rightarrow \qquad S_{ijkl} = C_{ijkl} \boxed{- P\delta_{ik}\delta_{jl}}$$

Associated with the second order term in the definition of the Lagrangian strain parameters

$$\eta_{ij} = \frac{1}{2}\left(u_{ij} + u_{ji} + \boxed{u_{li}u_{lj}}\right)$$

$P \neq 0$ ⇨ The leading order for energy is linear over displacements
The elastistic energy is of the next-to-leading order

Elasticity under finite pressure

[Wallace (1967), Baiko (2011), see also Marcus & Qiu (2009)]

$$\delta\mathcal{E} = \boxed{-P\delta_{ij}\eta_{ij}} + \frac{1}{2}C_{ijkl}\eta_{ij}\eta_{kl} = -P\delta_{ij}u_{ij} + \frac{1}{2}S_{ijkl}u_{ij}u_{kl}$$

$$\delta\sigma_{ij} = \frac{1}{2}B_{ijkl}\left(u_{kl} + u_{lk}\right)$$

$$B_{ijkl} = S_{ijkl} \boxed{- P\left(\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}\right)}$$

Associated with $-P\delta^{(2)}V$,
i.e. change of the volume (compression) in the second order of strain

$P \neq 0$ ⇨ The elastisic streses are linear over displacements

Elasticity under finite pressure

[Wallace (1967), Baiko (2011), see also Marcus & Qiu (2009)]

$$\delta E = \boxed{-P\delta_{ij}\eta_{ij}} + \frac{1}{2}C_{ijkl}\eta_{ij}\eta_{kl} = -P\delta_{ij}u_{ij} + \frac{1}{2}S_{ijkl}u_{ij}u_{kl}$$

$$\delta\sigma_{ij} = \frac{1}{2}B_{ijkl}\left(u_{kl} + u_{lk}\right)$$

$$P \neq 0 \Rightarrow \quad B_{ijkl} = S_{ijkl} - P\left(\delta_{il}\delta_{jk} - \delta_{ij}\delta_{lk}\right)$$

$$B_{ijkl} + B_{ilkj} = S_{ijkl} + S_{ijkl}$$

Uniform material

$$\delta f_i = \frac{\partial\delta\sigma_{ij}}{\partial x_j} = S_{ijkl}\frac{\partial^2\xi_k}{\partial x_j\partial x_l} = B_{ijkl}\frac{\partial^2\xi_k}{\partial x_j\partial x_l}$$

Elasticity under finite pressure

Example: barotropic material $P = P(\rho)$

$$K \stackrel{\text{def}}{=} -V_0 \frac{\partial P}{\partial V}, \quad \delta^{(1)} V = V_0 \, u_{ii} = V_0 \mathrm{div} \boldsymbol{\xi} \ \Rightarrow \delta^{(1)} P = -K \frac{\delta^{(1)} V}{V_0} = -K \, u_{ii}$$

$$-\delta^{(1)} P \delta_{ij} = \delta\sigma_{ij} = \frac{1}{2} B_{ijkl} \left(u_{kl} + u_{lk} \right) \Rightarrow \boxed{B_{ijkl} = K \delta_{ij} \delta_{kl}}$$

<u>The first order variation of energy:</u>

$$\delta^{(1)} \mathcal{E} = \frac{1}{V_0} \delta^{(1)} E = -P \frac{\delta^{(1)} V}{V_0} = -P u_{ii}$$

Energy per unit mass in deformed state

Volume per unit mass in non deformed state

$$\rho_0 = \frac{1}{V_0}$$

Elasticity under finite pressure

Example: barotropic material $P = P(\rho)$

$$K \overset{\text{def}}{=} -V_0 \frac{\partial P}{\partial V}, \quad \delta^{(1)} V = V_0\, u_{ii} = V_0 \mathrm{div}\boldsymbol{\xi} \;\Rightarrow \delta^{(1)} P = -K \frac{\delta^{(1)} V}{V_0} = -K\, u_{ii}$$

$$-\delta^{(1)} P \delta_{ij} = \delta\sigma_{ij} = \frac{1}{2} B_{ijkl} \left(u_{kl} + u_{lk}\right) \Rightarrow \boxed{B_{ijkl} = K \delta_{ij} \delta_{kl}}$$

<u>The second order variation of energy:</u>

$$\frac{1}{2} S_{ijkl} u_{ij} u_{kl} = \delta^{(2)} \mathcal{E} = \frac{1}{V_0} \left(-P \delta^{(2)} V + \boxed{\frac{K}{2\, V_0} \left(\delta^{(1)} V\right)^2} \right)$$

$$-\int_{V_0}^{V_0 + \delta V} \delta^{(1)} P \,\mathrm{dV}$$

$$\delta^{(2)} V = V_0 \left(\delta_{il} \delta_{jk} - \delta_{ij} \delta_{kl}\right) u_{ij}\, u_{kl}$$

$$\begin{aligned} S_{ijkl} &= -P \left(\delta_{il} \delta_{jk} - \delta_{ij} \delta_{kl}\right) + K \delta_{ij} \delta_{kl} \\ &= -P \left(\delta_{il} \delta_{jk} - \delta_{ij} \delta_{kl}\right) + B_{ijkl} \end{aligned}$$

Elasticity under finite pressure

Example: isotropic elastic material

$$B_{ijkl} = K\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \tfrac{2}{3}\delta_{ij}\delta_{kl}\right)$$

The same form as for $P = 0$

$$\begin{aligned} S_{ijkl} &= B_{ijkl} + P\left(\delta_{il}\delta_{jk} - \delta_{ij}\delta_{kl}\right) \\ &= (K - P)\,\delta_{ij}\delta_{kl} + \mu\delta_{ik}\delta_{jl} \\ &+ (\mu + P)\,\delta_{il}\delta_{jk} - \frac{2\mu}{3}\delta_{ij}\delta_{kl} \end{aligned}$$

Elasticity under finite pressure

Example: isotropic elastic material

$$B_{ijkl} = K\delta_{ij}\delta_{kl} + \mu\left(\delta_{ik}\delta_{jl} + \delta_{il}\delta_{jk} - \tfrac{2}{3}\delta_{ij}\delta_{kl}\right)$$

$$\begin{aligned}\delta\sigma_{ij} &= \frac{1}{2}B_{ijkl}\left(u_{kl} + u_{lk}\right) \\ &= K\delta_{ij}u_{ll} + \frac{\mu}{2}\left(u_{ik} + u_{ki} - \frac{2}{3}\delta_{ik}u_{ll}\right)\end{aligned}$$

Equation for variation of the stress tensor have standard form (same as for vanishing pressure at non-deformed state)

B_{ijkl} Seems to be the most useful for neutron star applications (allows to calculate stresses, but not the energies!!!)

S_{ijkl} Is useful for microphysical calculations [e.g. Baiko 2011]

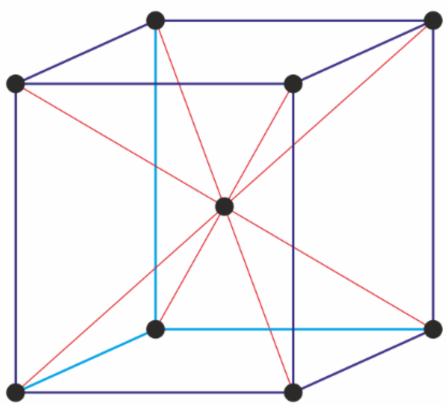
Basic model and scaling

[one component crust – all ions are equal]

$$\delta\sigma_{ij} = \frac{Z^2 e^2}{a} n\, \delta\tilde{\sigma}_{ij}\left(u_{ij}, \Gamma = \frac{Z^2 e^2}{aT}, \frac{T}{\hbar\omega_P}, ak_{\mathrm{TF}}, \ldots\right)$$

Point charges, TF screening: $\quad a = (4\pi n/3)^{-1/3}$

Ions form BCC lattice



(Arbitrary) uniform compression/expansion does not lead to breaking

(but can initiate nuclear reactions)

Beyond scope: Realistic (Jancovici 1962) electron screening [Baiko 2002]

Effects of free neutrons: induced interactions [Kobyakov&Pethick 2016]

Small deformations: Monocrystal

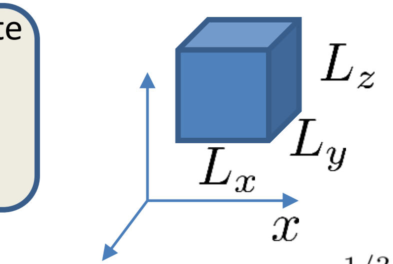
Fuchs (1936) (neglecting screening):

Very strong anisotropy

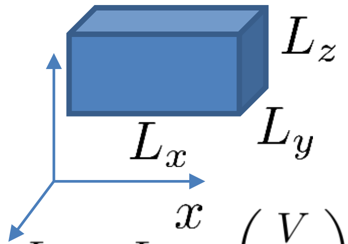
Volume conserving tension:

$$u_{xx} = \epsilon + \boxed{\frac{3}{2}\epsilon^2}$$
$$u_{yy} = u_{zz} = -\frac{1}{2}\epsilon$$

Allows to calculate B_{ijkl} because $\delta^{(2)}V = 0$

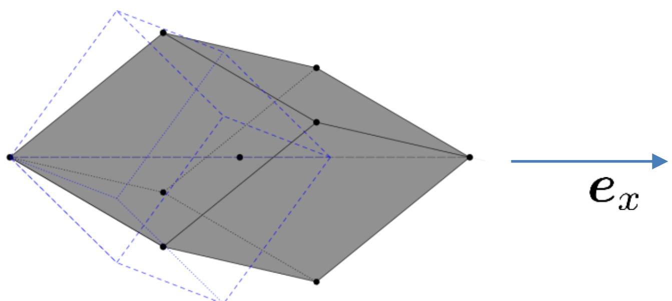


$L_x = L_y = L_z = V^{1/3}$



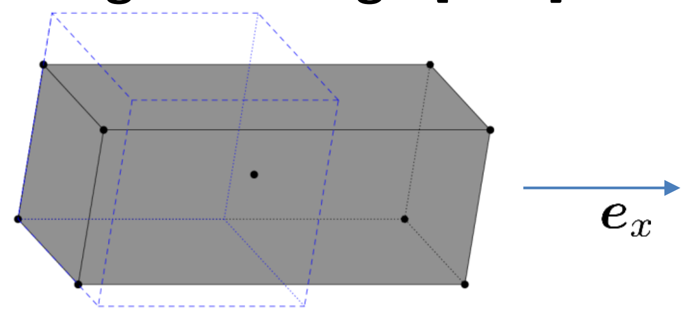
$L_y = L_z = \left(\frac{V}{L_x}\right)^{1/2}$

Along cube diagonal [111]



$$\delta\sigma_{xx} = 2\,c_{44}\epsilon \approx \boxed{0.366\epsilon}\frac{Z^2e^2}{a}n$$
$$\delta\sigma_{yy} = \delta\sigma_{zz} = -\frac{1}{2}\delta\sigma_{xx}$$

Along cube edge [100]



$$\delta\sigma_{xx} = (c_{12} - c_{11})\epsilon \approx \boxed{0.049\epsilon}\frac{Z^2e^2}{a}n$$
$$\delta\sigma_{yy} = \delta\sigma_{zz} = -\frac{1}{2}\delta\sigma_{xx}$$

Hidden symmetry of elasticity tensor

Uniform deformation at microphysical level

$$\boldsymbol{R} \to \boldsymbol{R}' = \boldsymbol{R} + \boldsymbol{\xi}(\boldsymbol{R}), \quad \xi_i = u_{ij} R_j$$

Change in energy (ion-ion interaction for example)

$$\delta \mathcal{E}'_{ion} = \frac{1}{2} \sum_{ions} Z_a Z_b e^2 \left(\frac{1}{|\boldsymbol{R} + \boldsymbol{\xi}(\boldsymbol{R})|} - \frac{1}{|\boldsymbol{R}|} \right)$$

Agrees with numerical results by Kozhberov (2019)

$$\frac{R_i}{R^3}\xi_i + \frac{3R_iR_k - R^2\delta_{ik}}{R^5}\xi_i\xi_k = \boxed{\frac{R_iR_j}{R^3}u_{ij}} + \boxed{\frac{3R_iR_k - R^2\delta_{ik}}{R^5}R_jR_l u_{ij}u_{kl}}$$

Contributes to S_{ijkl}, but note:

$$S_{ijij} = 0$$

For any Coulomb crystal (arbitrary structure and composition), neglecting ion motion

After summation over ions lead to term

$$-\sigma^0_{ij} V_0 \, u_{ij} = -P\mathrm{d}V$$

(if nondeformed lattice had symmetric stress tensor)

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Contributes to S_{ijkl}, but note:

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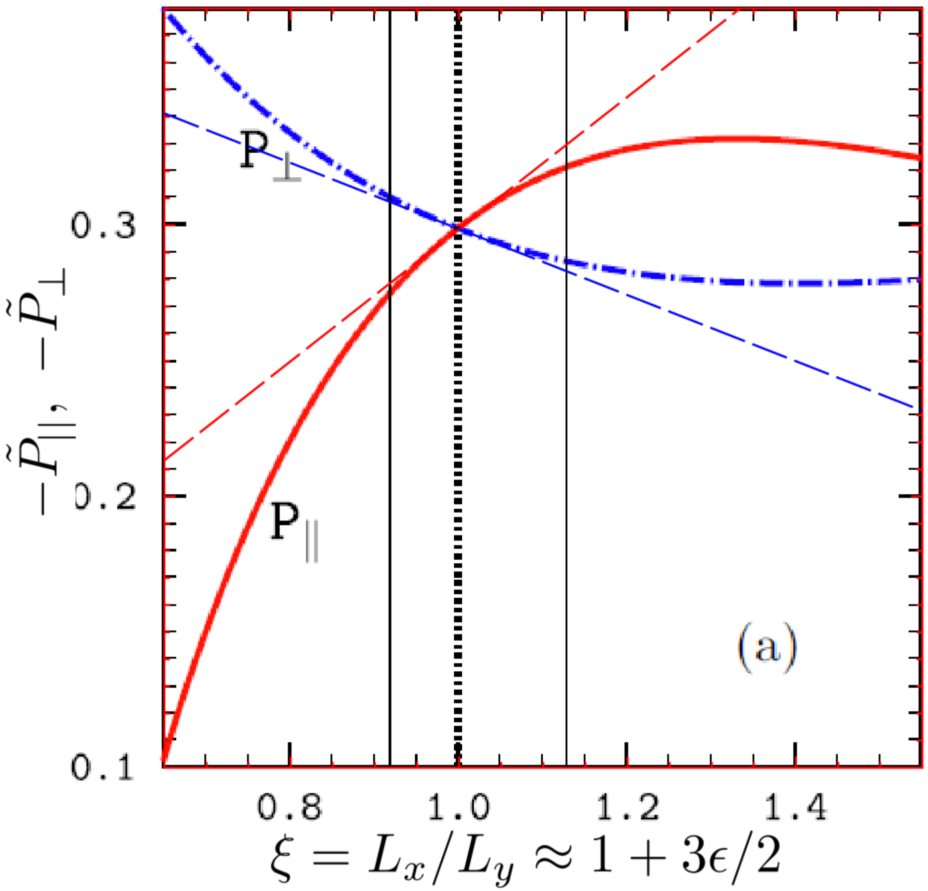
For any Coulomb crystal (arbitrary structure and composition), neglecting ion motion

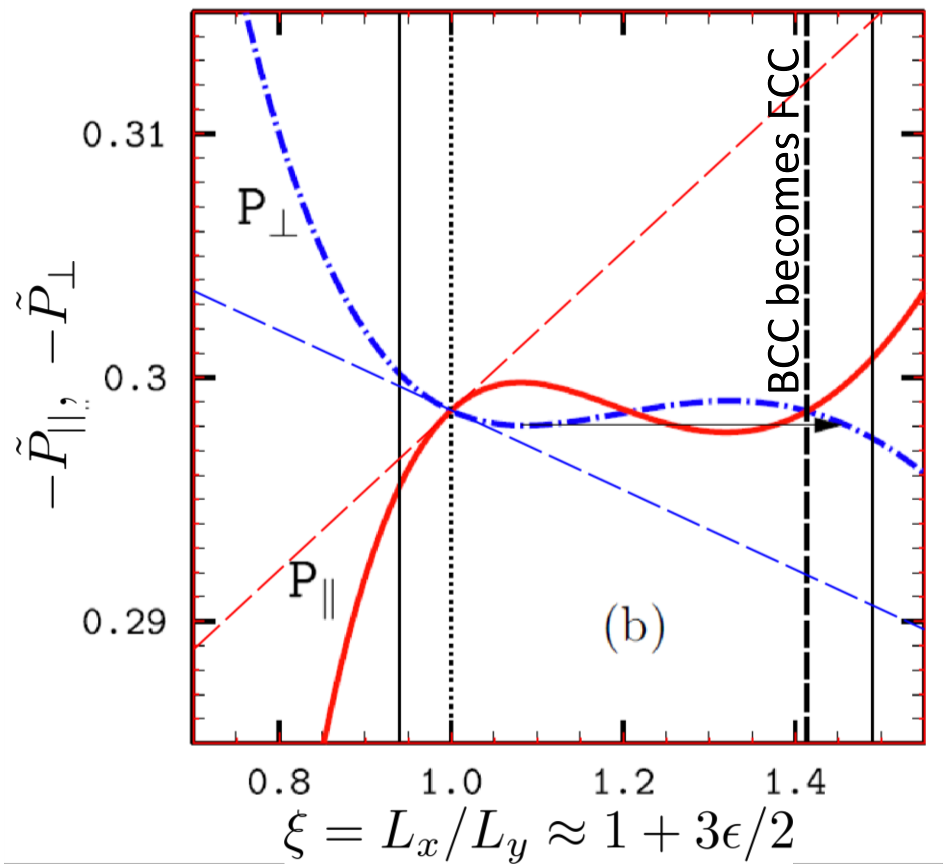
Large deformations: Monocrystal

[Baiko&Kozhberov 2017]

Along cube diagonal [111]



Along cube edge [100]



Stress is strongly nonlinear (at certain directions)

Breaking stress is anisotropic (note the difference in scales)

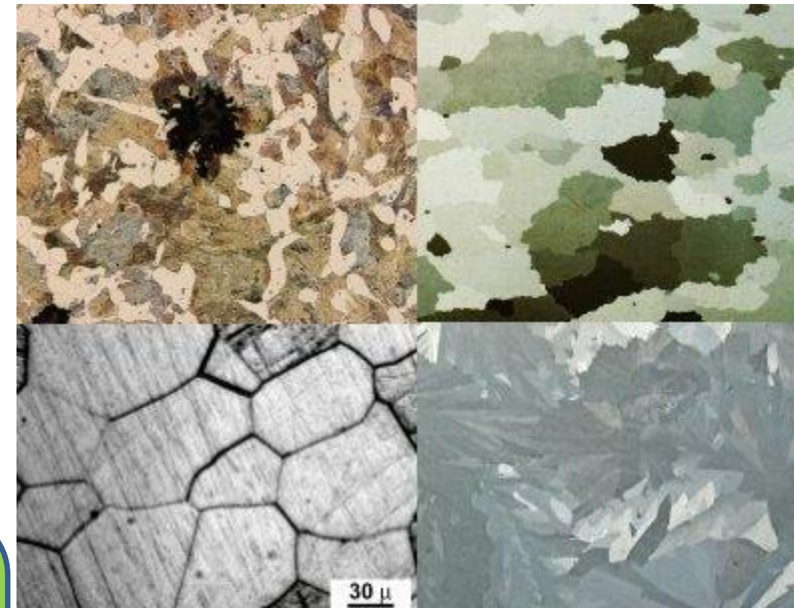
Small deformations: Polycrystal

Polycrystalline matter, made of large number of single crystals, should be isotropic.

$$\delta\sigma_{ij} = \mu_{\rm eff}\left(u_{ik} + u_{ki} - \frac{2}{3}\delta_{ij}u_{ll}\right) + K u_{ll}\delta_{ij}$$

Shear modulus

Compression modulus



[From Wikipedia]

Landau&Lifshitz, vol. 7: “The relation between the elastic properties of the whole crystal and those of components crystallites depends on actual form of the latter and the amount of correlation of their mutual orientation.”

Ogata&Ichimaru (1990):
(Uniform deformation=Voigt average)

$$\mu_{\rm eff}^{\rm V} = 0.120\frac{Z^2e^2}{a}n$$

Kobyakov&Pethick (2015):
(self consistent theory by Eshelby 1961)

$$\mu_{\rm eff}^{\rm sc} = 0.093\frac{Z^2e^2}{a}n$$

28% difference

Polycrystalline crust: Voigt average

Assumptions:
(1) uniform distribution of crystallite orientations
(2) uniform deformation within whole polycrystalline matter

$$\delta^{(2)}\mathcal{E} = \sum_c \frac{V_c}{2V} S^c_{ijkl} u_{ij} u_{kl} = \sum_c \frac{V_c}{2V} S_{mnop} R^c_{im} R^c_{jn} R^c_{ko} R^c_{lp} u_{ij} u_{kl} = S^V_{ijkl} u_{ij} u_{kl}$$

Rotation matrix, required to rotate crystal axis to the lab system

$$\Downarrow$$

$$S^V_{ijkl} = \langle S_{mnop} R^c_{im} R^c_{jn} R^c_{ko} R^c_{lp} \rangle$$

$$\Downarrow \quad R_{ik} R_{il} = \delta_{kl}$$

Following convolutions are invariants (see, e.g. D. Blaschke 2017)

$$S^V_{iijj} = \langle S_{mnop} R_{im} R_{in} R_{jo} R_{jp} \rangle = \langle S_{mnop} \delta_{mn} \delta_{op} \rangle = S_{iijj}$$

$$S^V_{ijij} = \langle S_{mnop} R_{im} R_{jn} R_{io} R_{jp} \rangle = \langle S_{mnop} \delta_{mo} \delta_{np} \rangle = S_{ijij}$$

Voigt average gives an upper limit for elastic tensor

(nonunifrom deformation of crystallites, in principle, can reduce the energy)

Polycrystalline crust: Voigt average

Assumptions:
(1) uniform distribution of crystallite orientations
(2) uniform deformation within polycrystalline

$$\delta^{(2)}\mathcal{E} = \sum_c \frac{V_c}{2V} S^c_{ijkl} u_{ij} u_{kl} = \sum_c \frac{V_c}{2V} S_{mnop} R^c_{im} R^c_{jn} R^c_{ko} R^c_{lp} u_{ij} u_{kl} = S^V_{ijkl} u_{ij} u_{kl}$$

Rotation matrix, required to rotate crystal axis to the lab system

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Following convolutions are invariants (see, e.g. D. Blaschke 2017)

$$S^V_{iijj} = \langle S_{mnop} R_{im} R_{in} R_{jo} R_{jp} \rangle = \langle S_{mnop} \delta_{mn} \delta_{op} \rangle = S_{iijj}$$

$$S^V_{ijij} = \langle S_{mnop} R_{im} R_{jn} R_{io} R_{jp} \rangle = \langle S_{mnop} \delta_{mo} \delta_{np} \rangle = S_{ijij}$$

For Coulomb crystals (neglecting ion motion): $S_{ijij} = 0 \;\Rightarrow\; S^V_{ijij} = 0$

(can be also shown in the same way as for monocrystal, by uniform deformation of polycrystal)

Polycrystalline crust: Voigt average

Isotropic elastic tensor:

$$B^V_{ijkl} = \lambda\delta_{ij}\delta_{kl} + 2\mu^V_{\rm eff}\left(\delta_{ik}\delta_{jl} - \delta_{il}\delta_{jk}\right), \quad K = \lambda + \frac{2}{3}\mu^V_{\rm eff}$$

$$\Downarrow$$

$$B^V_{ijij} = 3\lambda + 12\mu^V_{\rm eff}$$

For Coulomb crystals (neglecting ion motion):

$$B^V_{ijij} = S^V_{ijij} = 0 \;\Rightarrow\; \lambda = -4\,\mu^V_{\rm eff};\;\; K = -\frac{10}{3}\mu^V_{\rm eff}$$

$$E^M \propto \frac{n}{a_{\rm e}} \propto n^{4/3} \Rightarrow P = \frac{1}{3}E,\;\; K = n\frac{{\rm d}P}{{\rm d}n} = \frac{4}{9}E^M$$

$$\boxed{\mu^V_{\rm eff} = -\frac{2}{15}E^M}$$

For any Coulomb crystal
(arbitrary structure and composition)

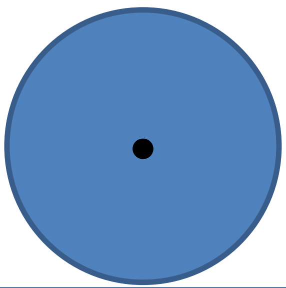
Small deformations: Polycrystal

$$\mu_{\rm eff}^{V} = -\frac{2}{15} E^{M}$$

For any Coulomb crystal
(arbitrary structure and composition)

Ion sphere model:

$$E^{\rm M} = -\frac{9}{10}\frac{Z^2e^2}{a}n, \quad a = \left(\frac{3}{4\pi n}\right)^{1/3}$$



$$\mu_{\rm eff}^{\rm V} = \frac{3}{25}\frac{Z^2e^2}{a}n = 0.12\frac{Z^2e^2}{a}n$$

Multicomponent crystal: Linear mixing rule

$$E^{\rm M} = -\frac{9}{10}\sum_i \frac{Z_i^{5/3}e^2}{a_e}n_i, \quad a_e = \left(\frac{3}{4\pi n_e}\right)^{1/3}$$

$$\mu_{\rm eff}^{\rm V} = \frac{3}{25}\sum_i \frac{Z_i^{5/3}e^2}{a_e}n_i = 0.12\sum_i \frac{Z_i^{5/3}e^2}{a_e}n_i$$

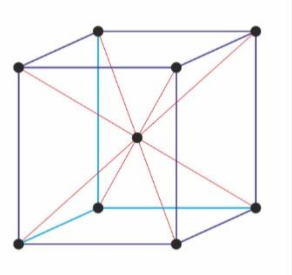
For arbitrary structure and composition of crystallites

Small deformations: Polycrystal

$$\mu_{\text{eff}}^{V} = -\frac{2}{15} E^{M}$$

For any Coulomb crystal
(arbitrary structure and composition)

bcc lattice:



$$E^{\mathrm{M}} = -\zeta \frac{Z^2 e^2}{a} n, \quad a = \left(\frac{3}{4\pi n}\right)^{1/3}, \quad \zeta = 0.89592925568$$

0.1194572 [Baiko 2011]

$$\mu_{\text{eff}}^{\mathrm{V}} = \frac{2\,\zeta}{15} \frac{Z^2 e^2}{a} n = 0.11945723409 \frac{Z^2 e^2}{a} n$$

Two component ordered crystal with BCC lattice

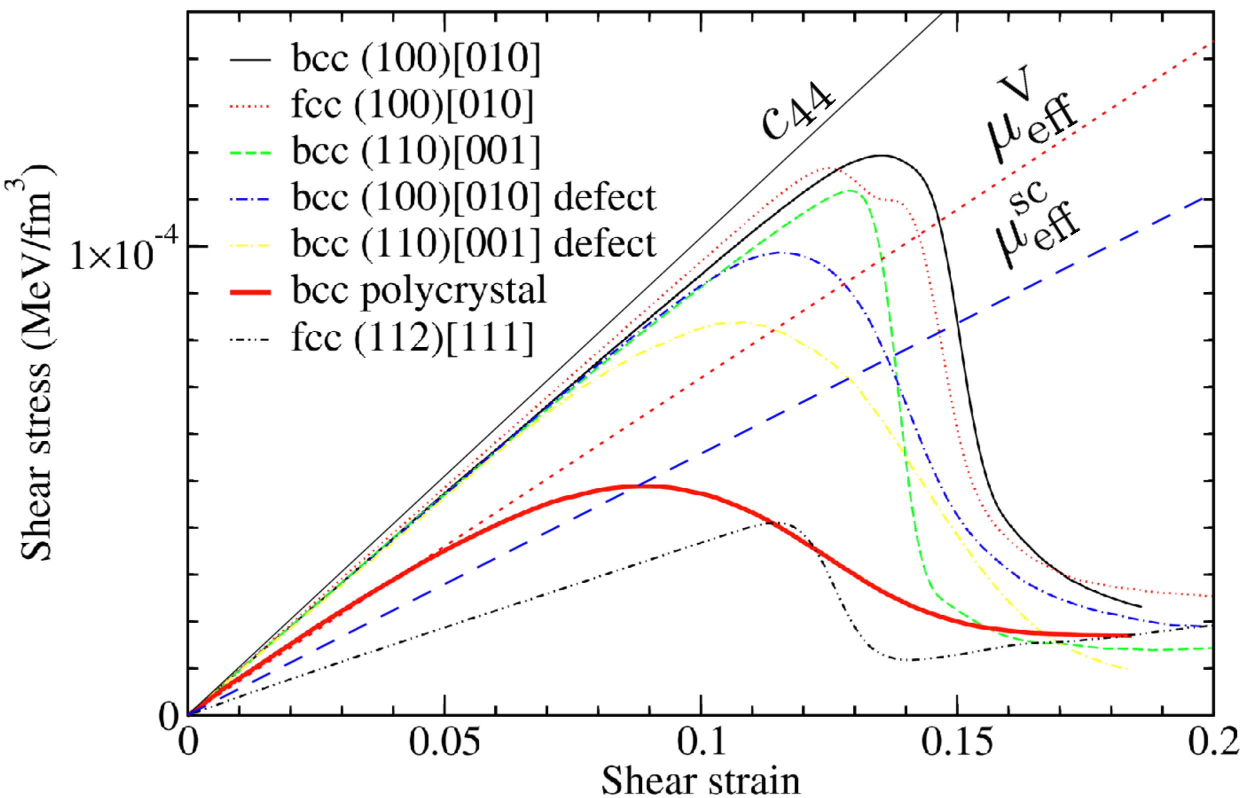
$$E^{\mathrm{M}} = -\zeta_M \frac{Z_1^2 e^2}{a} n, \quad a = \left(\frac{3}{4\pi n}\right)^{1/3}, \quad \zeta_M = 0.3492518 \left(1 + \frac{Z_1^2}{Z_2^2}\right) + 0.197425 \frac{Z_1}{Z_2}$$

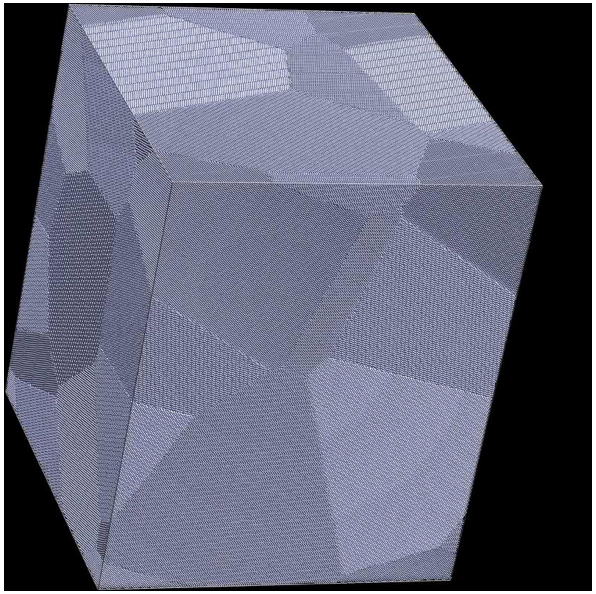
[Kozhberov, 2019]

$$\mu_{\text{eff}}^{\mathrm{V}} = \left[0.0465669 \left(1 + \frac{Z_1^2}{Z_2^2}\right) + 0.0263234 \frac{Z_1}{Z_2}\right] \frac{Z_1^2 e^2}{a} n = \frac{2\,\zeta_M}{15} \frac{Z^2 e^2}{a} n$$

Small deformations: Polycrystal

Numerical experiment: MD simulations by Horowitz&Kadau (2009) for shear deformations





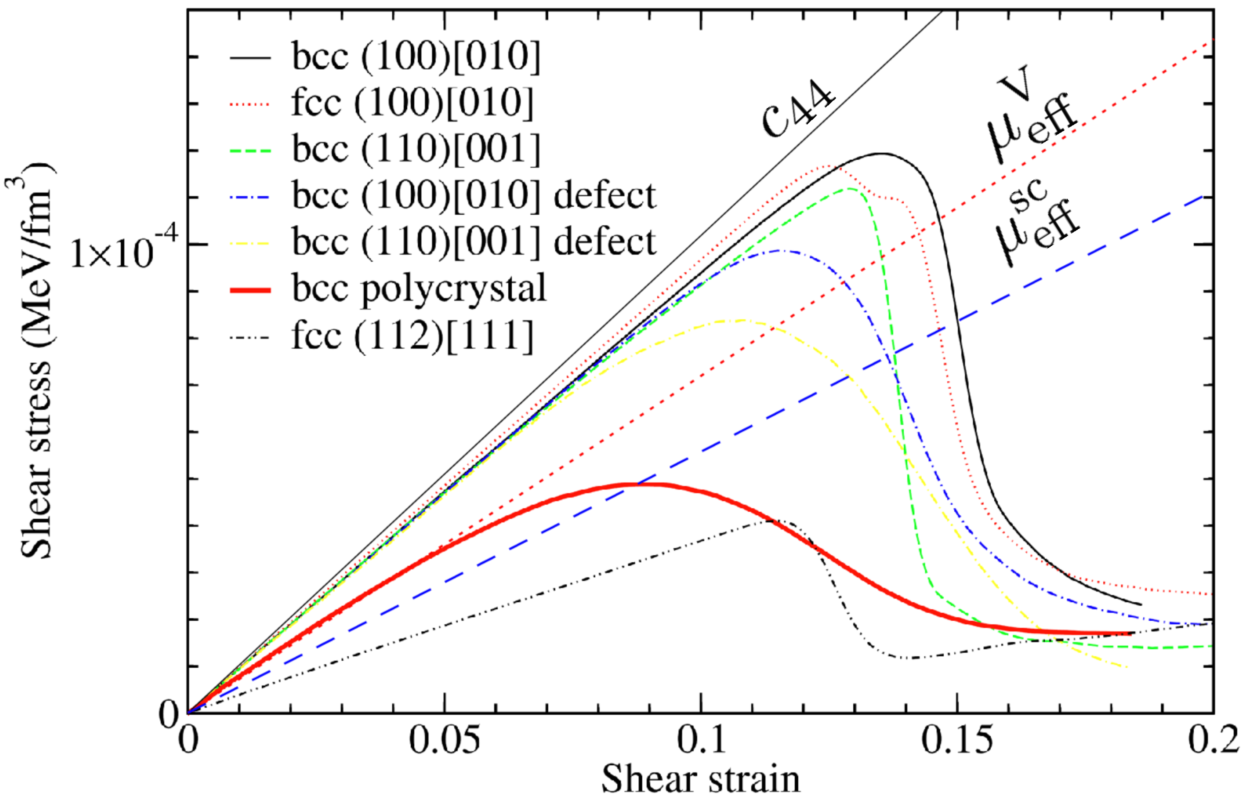
Movie and original figure from Horowitz&Kadau (2009)

Shear stress is almost linear for monocrystal

Effective shear modulus is rather uncertain

Breaking strain&stress

Numerical experiment: MD simulations by Horowitz&Kadau (2009)
[shear deformations]



Fractures and voids does not appear (Horowitz&Kadau, 2009)

Monocrystal

Breaking strain:

$$\epsilon_{\rm b} \sim 0.1$$

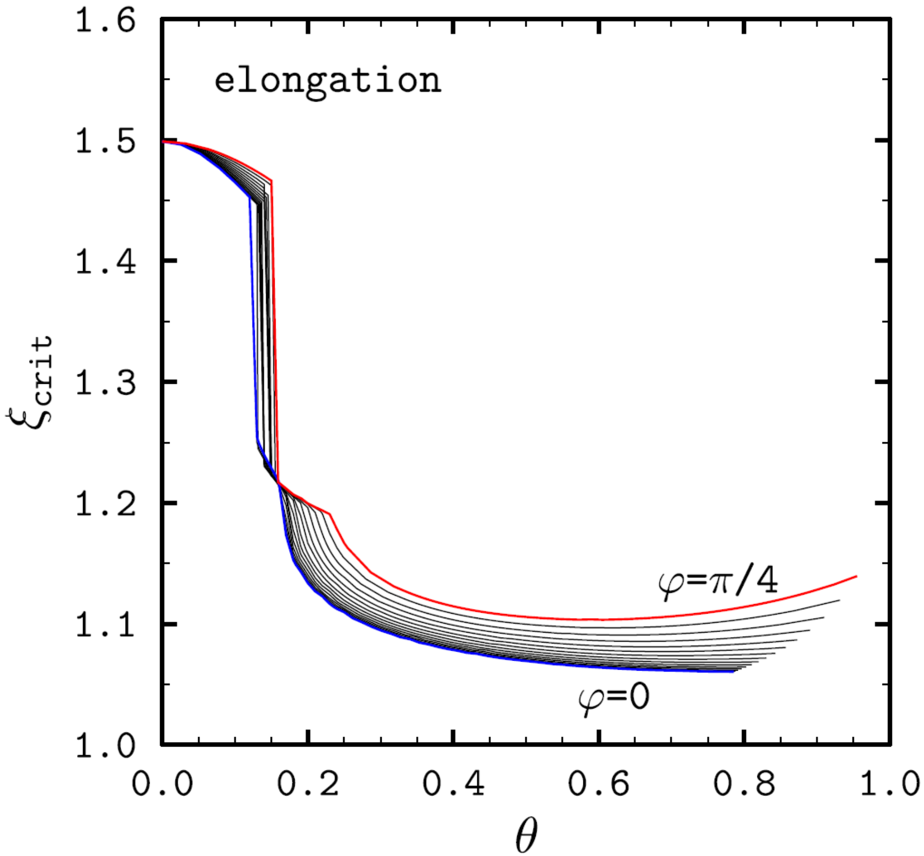
Breaking stress:

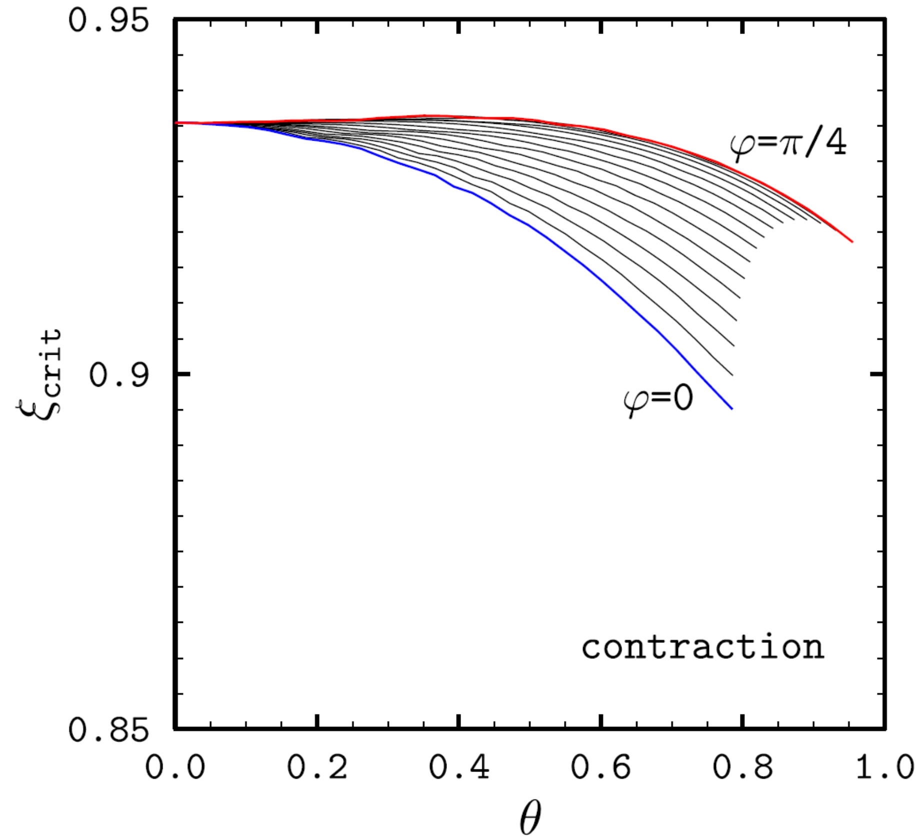
$$\Delta\sigma_{\rm b} \sim c_{44}\epsilon_{\rm b}$$

Polycrystal: breaking strain and stress are moderately reduced

Breaking strain&stress

Semianalitic approach: appearance of the unstable modes
[Baiko&Kozhberov 2017, Baiko&AIC 2018]

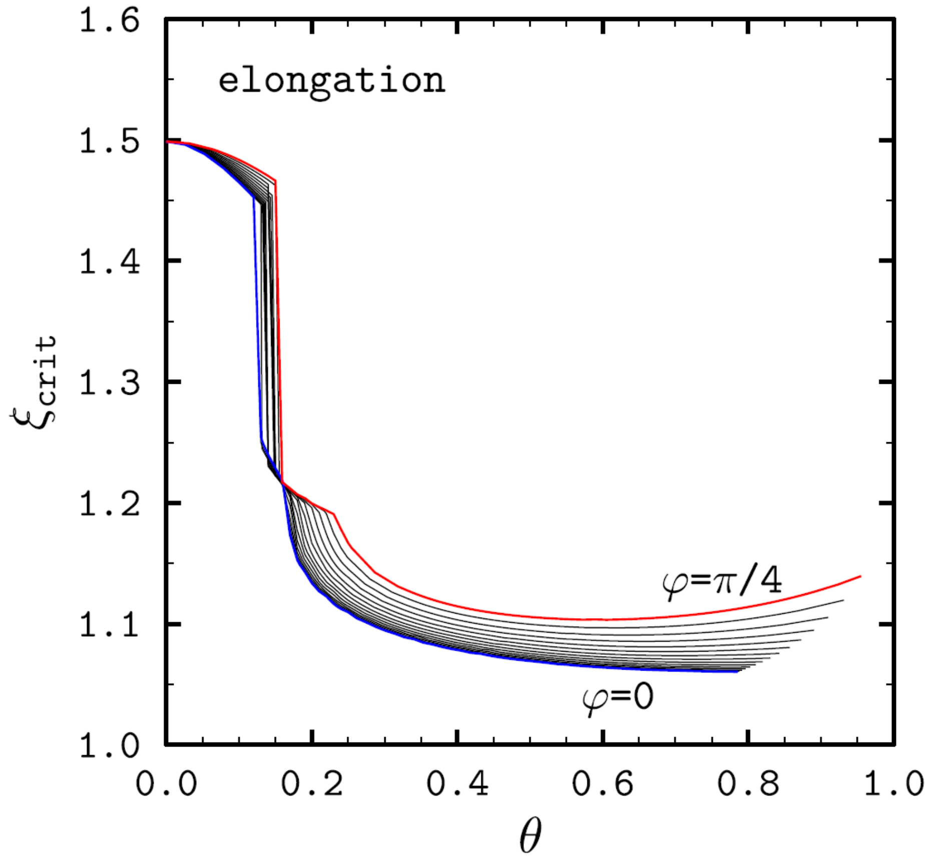


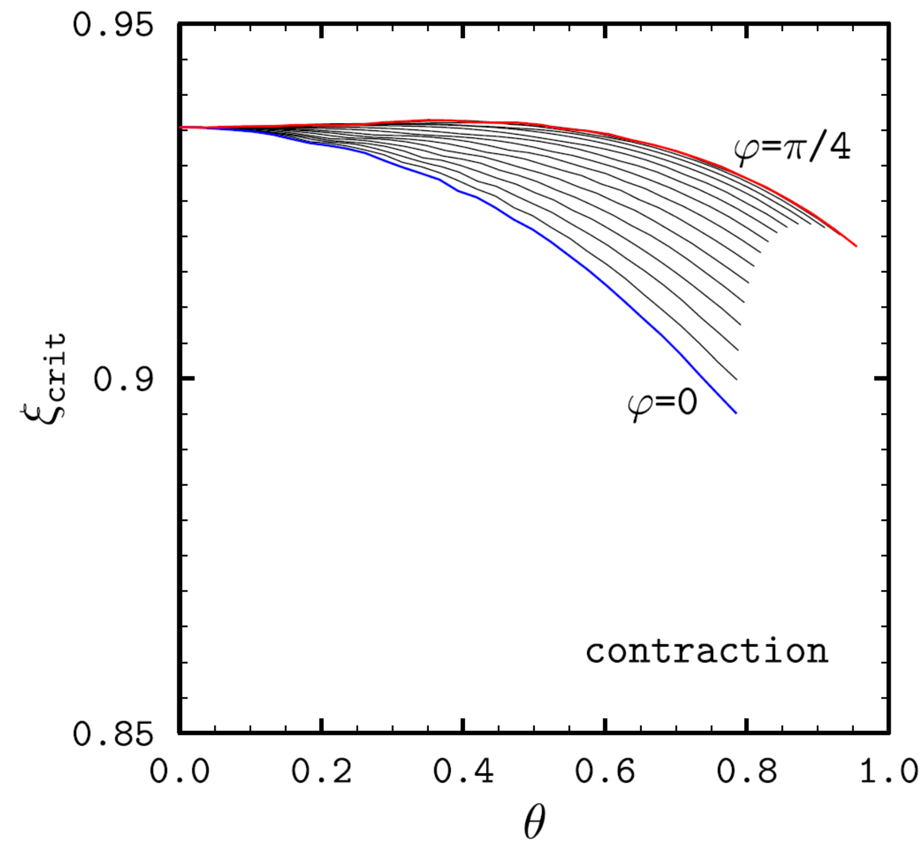


Critical deformation of perfect crystals is strongly anisotropic
(the same holds true for critical stress tensor and elastic energy)

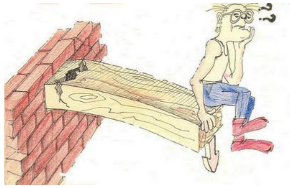
Breaking strain&stress

Semianalitical approach: appearance of the unstable modes
[Baiko&Kozhberov 2017, Baiko&AIC 2018]

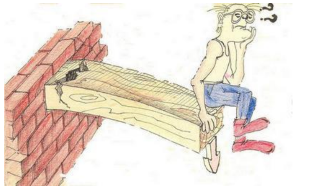




Polycrystalline matter should break when crystallite at the weakest orientation breaks $\epsilon_{\rm crit} \lesssim 0.04$



Part I: Summary



1. The stress-strain relation can be described by tensor B_{ijkl}.
   It has Voigt symmetry $$B_{ijkl} = B_{jikl} = B_{klij}$$
2. Elasticity tensor for Coulomb system have additional symmetry
$$B_{ikik} = S_{ikik} = 0$$
3. Elastic properties of polycrystalline matter are rather uncertain (~28% difference). The upper limit is given by the Voigt averaged shear modulus, which depends only on Coulomb (Madelung) energy.
$$\mu_{\rm eff}^{\rm V} = -\frac{2}{15} E^{\rm M} \approx 0.12 \sum_i \frac{Z_i^{5/3} e^2}{a_e} n_i$$
4. Uniform compression/expansion does not lead to breaking. Critical deformation is strongly anisotropic for monocristals. Critical deformation for polycrystalline matter $\boxed{\epsilon_{\rm crit} \lesssim 0.04}$

Part II: Nuclear reaction in strongly coupled plasmas

$$\boxed{\boxed{A + B \to O^*} \to C + D}$$

Well studied in literature
[Salpeter (1954), …]

The reaction rate

$$\boxed{R_{A+B\to O^*}} = \boxed{F^{\mathrm{scr}}_{A+B\to O^*}}\boxed{R^{\mathrm{th}}_{A+B\to O^*}}$$

Enhancement factor

Thermonuclear reaction rate
(in rarefied plasma)

Required for astrophysical applications

What is the reaction rate for

$$A + B \to C + D$$

In a stellar conditions?
(in strongly coupled plasmas)

?

<u>A bit of terminology</u>: The enhancement some times referred as ‘electron screening’, but the main contribution is associated with correlations between ions

Nuclear reaction in strongly coupled plasmas

$$A + B \to O^* \to C + D$$

Rate of the reactions via compound nucleus

$$\boxed{R_{A+B\to O^*}}\ \boxed{b_{O^*\to C+D}} = R_{A+B\to C+D}$$

Well studied in literature

[Salpeter (1954) …]

The branching factor

Obviously unaffected by plasma screening

(as far as nuclear scales are much shorter than plasma scales)

$$R_{A+B\to O^*} = F^{\rm scr}_{A+B\to O^*} R^{\rm th}_{A+B\to O^*}$$

$$\begin{aligned} R_{A+B\to C+D} &= b_{O^*\to C+D}\ F^{\rm scr}_{A+B\to O^*} R^{\rm th}_{A+B\to O^*} \\ &= F^{\rm scr}_{A+B\to O^*} R^{\rm th}_{A+B\to C+D} \end{aligned}$$

It is highly likely, that the resulting enhancement factor is the same as for formation of the compound nucleus

Nuclear reaction in strongly coupled plasmas

$$A + B \to O^* \to C + D$$

Rate of the reactions via compound nucleus

$$R_{A+B\to O^*} \quad b_{O^*\to C+D} = R_{A+B\to C+D}$$

Calder et al. (2007) [ApJ, 656, 313]:

These reaction rates leads to violation of nuclear statistical equilibrium (detailed balance)…

"Patch" solution:
"A favored reaction direction must be chosen and the reverse rate computed from its screened rate. The choice is apparent in the case of photodisintegrating reverse reactions …"

That is the reason of the problem? Is the patch applicable?

Nuclear reaction in strongly coupled plasmas
The detailed balance

$$A + B \to O^* \to C + D$$

Rate of the reactions via compound nucleus

$$\boxed{R_{A+B\to O^*}}\ \boxed{b_{O^*\to C+D}} = R_{A+B\to C+D}$$

Studied in "plasma enhancement" literature

The branching factor
Obviously unaffected by plasma screening
(as far as nuclear scales are much shorter than plasma scales)

$$R_{A+B\to O^*} = F^{\mathrm{scr}}_{A+B\to O^*} R^{\mathrm{th}}_{A+B\to O^*}$$

??? Which factor is wrong ???

Nuclear reaction in strongly coupled plasmas
The detailed balance

$$A + B \to O^* \to C + D$$

<u>Rate of the reactions via compound nucleus</u>

$$\boxed{R_{A+B\to O^*}}\ \boxed{b_{O^*\to C+D}} = R_{A+B\to C+D}$$

Studied in "plasma enhancement" literature

The branching factor
Obviously unaffected by plasma screening

(as far as nuclear scales are much shorter than plasma scales)

Nuclear reaction in strongly coupled plasmas
The detailed balance

$$A + B \to O^* \to C + D$$

The branching factor

Obviously unaffected by plasma screening

(as far as nuclear scales are much shorter than plasma scales)

$$^{12}\mathrm{C}+^{12}\mathrm{C},\ \rho = 5\times 10^9\ \mathrm{g/cm^{-3}},\ T = 10^8\ \mathrm{K}$$

The plasma scale: $a = \left(\frac{3}{4\pi n}\right)^{1/3} \sim 100\ \mathrm{fm}$

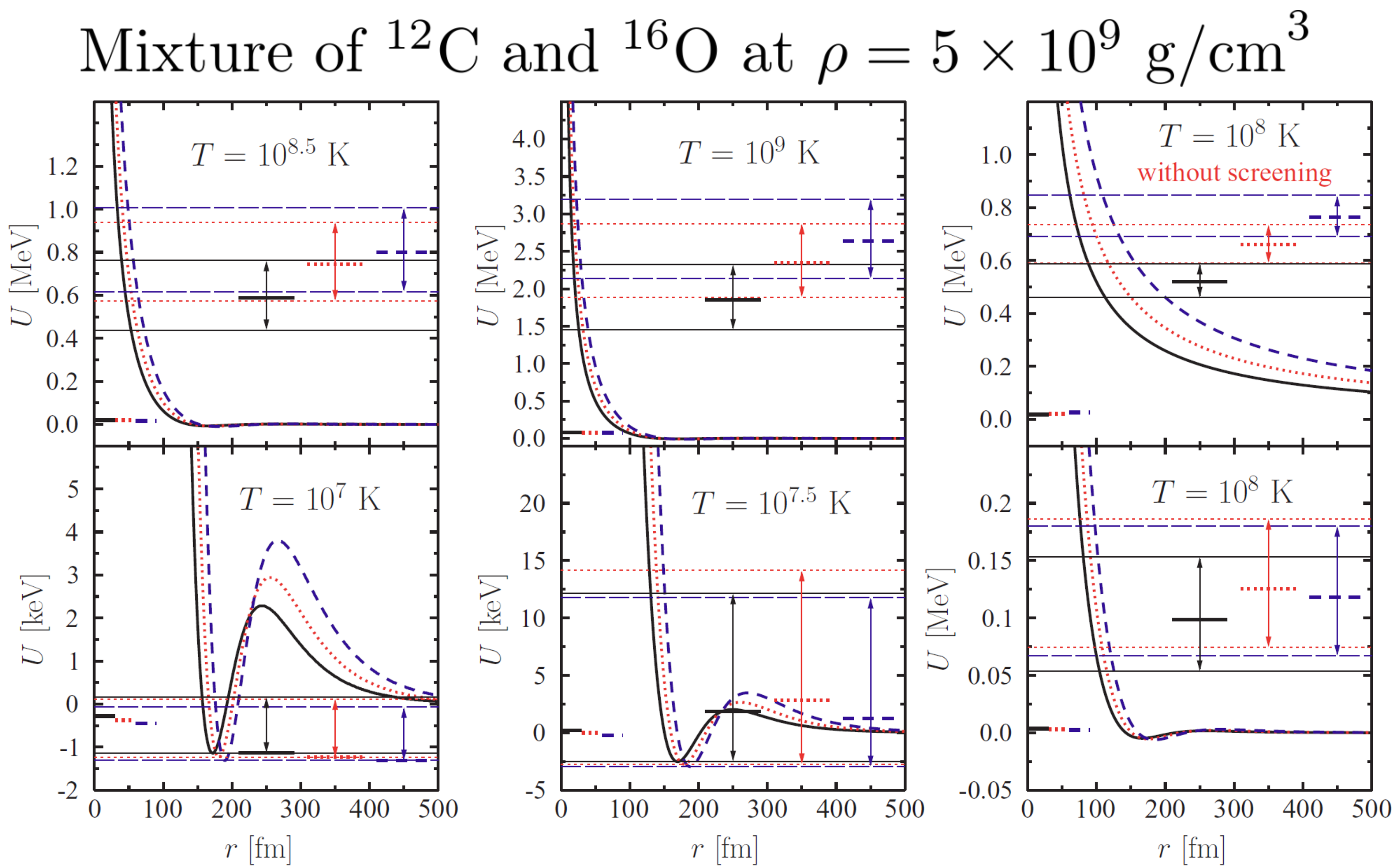
The largest nuclear scale :
The tunneling length for
Gamow peak ions

$$a_{\mathrm{pk}} = \left(\frac{2\hbar^2 e^2}{\pi^2}\,\frac{Z^2}{\mu T^2}\right)^{1/3} \sim 100\,\mathrm{fm}$$

The branching factor can be affected by plasma!

Why the branching factor can be affected?

The plasma screening affects the internuclear potential ⇒ The tunneling probability is affected



[from AIC & DeWitt 2009]

How to calculate branching factor correctly?

Take into account the plasma screening while calculating the widths of the reaction channels,
applying the same formalism as for compound nucleus formation

The width of the n-th decay channel of compound nucleus γ_n $\Rightarrow$ $\tilde{\gamma}_n = f_n^{\mathrm{q}} \gamma_n$

The plasma correction factor for tunneling probability

Total width $\Gamma = \sum_n \gamma_n$ $\Rightarrow$ $\tilde{\Gamma} = \sum_n \tilde{\gamma}_n$

Branching factor $b_n = \gamma_n / \Gamma$ $\Rightarrow$ $\tilde{b}_n = \tilde{\gamma}_n / \tilde{\Gamma}$

Reaction rate $A + B \to O^* \to C + D$

$$R_{A+B\to C+D} = \boxed{\tilde{b}_{O^*\to C+D}} \, F^{\mathrm{scr}}_{A+B\to O^*} R^{\mathrm{th}}_{A+B\to O^*}$$

The enhancement factor for nuclear reaction rates

Kushnir, Waxman & Chugunov [MNRAS **486** (2019), 449; arXiv:1805.08788]

$$A + B \to O^* \to C + D$$

$$R_{A+B\to C+D} \quad = \quad \tilde{b}_{O^*\to C+D}\, F^{\rm scr}_{A+B\to O^*} R^{\rm th}_{A+B\to O^*}$$

$$F^{\rm scr}_{A+B\to O^*} = f^{\rm cl}_{A+B\to O^*}\; f^{\rm q}_{A+B\to O^*}$$

Classical enhancement factor (increase of number of close encounters, screening in classically allowed region)

[Salpeter (1954), Dewitt et al. (1973), …]

$$f^{\rm cl}_{A+B\to O^*} = \exp\left[\frac{\mu^C(A) + \mu^C(B) - \mu^C(O)}{T}\right]$$

Quantum correction (plasma effect on the tunneling probability, screening at classically forbidden region)

$$f^{\rm q}_{A+B\to O^*} = f^{\rm q}_{O^*\to A+B}$$

$$F^{\rm scr}_{A+B\to C+D} \quad = \quad f^{\rm cl}_{A+B\to O^*} f^{\rm q}_{A+B\leftrightarrow C+D}$$

$$f^{\rm q}_{A+B\leftrightarrow C+D} \quad = \quad f^{\rm q}_{O^*\to A+B} f^{\rm q}_{O^*\to C+D} \frac{\Gamma}{\tilde{\Gamma}}$$

In agreement with the detailed balance principle

The enhancement factor for nuclear reaction rates

[simplified version for strongly exothermic reactions]

$$A + B \to O^* \to C + D$$

Only one channel (n=0) is associated with long tunneling
[for example, reaction with high Q value]

Neglect quantum correction for other channels

Long distance tunneling leads to small width for n=0 channel

$$\left.\begin{array}{l} f_n^{\mathrm{q}} \approx 1 \;\Leftrightarrow\; \tilde{\gamma}_n = \gamma_n \\[2ex] \tilde{\gamma}_0 \ll \gamma_n \end{array}\right\} \Rightarrow \begin{array}{rcl} \tilde{b}_0 & \approx & f_0^{\mathrm{q}}\, b_0 \\ \tilde{b}_n & \approx & b_n \\ \tilde{\Gamma} & \approx & \Gamma \end{array}$$

$$\begin{aligned} f^{\mathrm{q}}_{A+B\leftrightarrow C+D} &= f^{\mathrm{q}}_{O^*\to A+B} f^{\mathrm{q}}_{O^*\to C+D} \frac{\Gamma}{\tilde{\Gamma}} \approx f^{\mathrm{q}}_{O^*\to A+B} \\ F^{\mathrm{scr}}_{A+B\to C+D} &= f^{\mathrm{cl}}_{A+B\to O^*} f^{\mathrm{q}}_{A+B\leftrightarrow C+D} \approx F^{\mathrm{scr}}_{A+B\to O^*} \end{aligned}$$

The enhancement factor for high-Q reactions is the same as for reaction of compound nucleus formation

(NOTE: it is not holds true for reverse reaction)

Part II: Summary

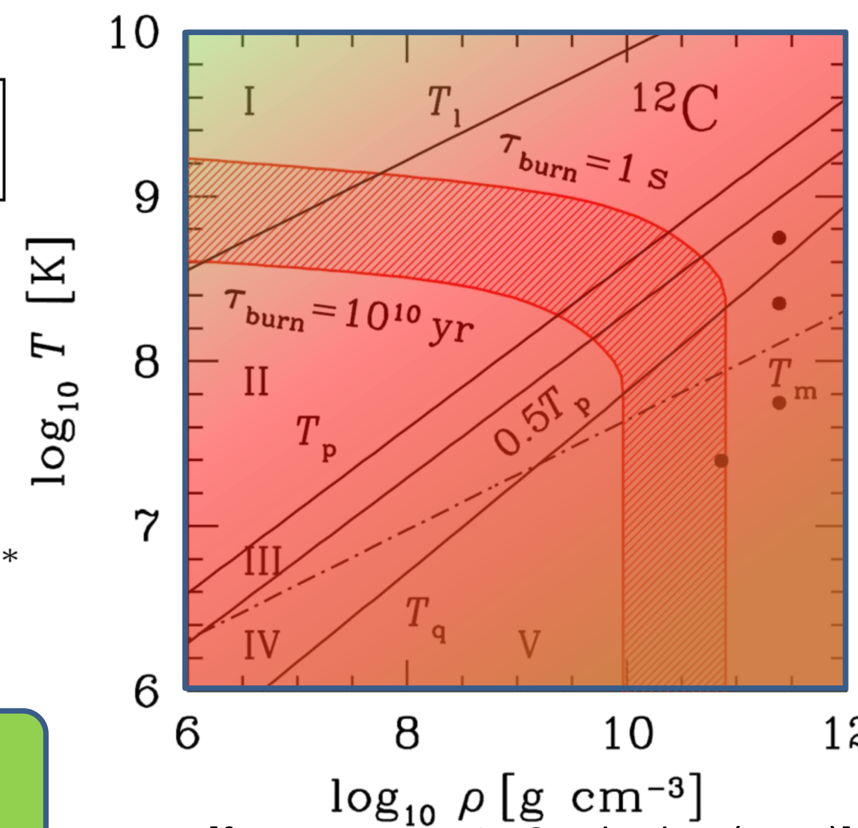
- Plasma screening affects internuclear potential and thus tunneling probability. This effect should be included into calculations consistently: not only for formation of compound nucleus, but also for decay rates and branching factors.

- The enhancement factor should be consistent with thermodynamic model [Kushnir, Waxman & AIC, MNRAS **486** (2019), 449]

$$f^{\rm cl}_{A+B\to O^*} = \exp\left[\frac{\mu^C(A)+\mu^C(B)-\mu^C(O)}{T}\right]$$

- For strongly exothermic reactions

$$\begin{aligned} F^{\rm scr}_{A+B\to C+D} &\approx F^{\rm scr}_{A+B\to O^*} \\ F^{\rm scr}_{C+D\to A+B} &= f^{\rm cl}_{C+D\to O^*} f^{\rm q}_{A+B\to O^*} \\ &\neq F^{\rm scr}_{C+D\to O^*} \end{aligned}$$



[from AIC, DeWitt & Yakovlev (2007)]

The “patch” solution does not holds true

Takeaway messages

1. Elastic properties of polycrystalline matter are rather uncertain (~28% difference). The upper limit is given by the Voigt averaged shear modulus, which depends only on Coulomb (Madelung) energy.
$$\mu_{\rm eff}^{\rm V} = -\frac{2}{15} E^{\rm M} \approx 0.12 \sum_i \frac{Z_i^{5/3} e^2}{a_e} n_i$$
2. Uniform compression/expansion does not lead to breaking. Critical deformation for polycrystalline matter
$$\epsilon_{\rm crit} \lesssim 0.04$$ [Baiko & AIC, 2018]
3. The enhancement factor for nuclear reactions should be consistent with thermodynamic model [Kushnir, Waxman & AIC (2019)]. For exothermic reactions:
$$\begin{aligned} F^{\rm scr}_{A+B\to C+D} &\approx F^{\rm scr}_{A+B\to O^*} \\ F^{\rm scr}_{C+D\to A+B} &= f^{\rm cl}_{C+D\to O^*} f^{\rm q}_{A+B\to O^*} \\ &\neq F^{\rm scr}_{C+D\to O^*} \end{aligned}$$