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Supplementary Information for "High partial auxeticity in simple model with Yukawa interactions induced by nanochannels in [111]-direction"

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1. Used nomenclature

The signs used in the manuscript are shown below

- N – the number of particles
- N_{HS} – the number of particles forming inclusion
- N_Y – the number of 'Yukawa' particles
- n – the number of fcc cells on the edge of the system
- c – the concentration of the nanoinclusion particles
- σ – the particles' diameter
- κ^{-1} – the Debye's screening length
- ϵ – the contact potential
- $\beta = 1/(k_B T)$
- k_B – the Boltzmann constant
- T – the temperature
- r_{ij} – distance between i-th and j-th particle
- S_{ijkl} – component of elastic compliance tensor
- ε_{ij} – component of strain tensor
- V_p – equilibrium volume of the system
- P – pressure
- $p^* \equiv \beta P \sigma^3$ – reduced pressure
- $\mathbf{h}$ – the box matrix
- $\mathbf{h}_0 \equiv \langle \mathbf{h} \rangle$ – the reference box matrix
- I – identity matrix
- δ_{ij} – the Kronecker delta
- n_i – the i-component of a unit vector in the direction of the applied stress
- m_i – the i-component of a unit vector in the direction in which the reaction of the system is observed.
- ν_{nm} – the Poisson's ratio
- χ – the degree of auxeticity

In this paper Voigt's notation and Einstein's summation are used.

2. Computations of the elastic compliances

The Lagrangian strain tensor can be expressed as [1]:

$$\varepsilon_{ij} \equiv \left(\partial_i u_j + \partial_j u_i + \sum_k \partial_i u_k \partial_j u_k \right) / 2 \,, \tag{1}$$

where $u_i \equiv x_i - X_i$ is the displacement vector and X_i, x_i describe respectively the undeformed state and the state under the deformation [1]. Under constant isotropic pressure (P) the expansion of the change of free enthalpy (Gibbs free energy), ΔG, caused by deformation of a crystal has the form [2]:

$$\Delta G = \frac{1}{2} V_p B_{ijkl} \varepsilon_{ij} \varepsilon_{kl} + ... \tag{2}$$

where B_{ijkl} are the components of the elastic constants tensor at fixed temperature and pressure P (the Einstein's summations is used). Under the isotropic pressure conditions, $\sigma_{ij} \equiv -P\delta_{ij}$, the elastic constans B_{ijkl} form the relation between the components of the strain tensor ε_{kl} and the stress tensor σ_{ij} [3] (the Hooke's law):

$$\Delta\sigma_{ij} = B_{ijkl} \varepsilon_{kl}, \tag{3}$$

where $\Delta\sigma_{ij} \equiv \sigma_{ij} + P\delta_{ij}$. By inversion, the above reads:

$$\varepsilon_{ij} = S_{ijkl} \Delta\sigma_{kl}, \tag{4}$$

where S_{ijkl} is the elastic compliance tensor, a fourth-rank tensor which remains unchanged when replacing *i*-*j*, *k*-*l* and *ij*-*kl*. The elastic compliances are related to the elastic constants tensor elements by the following equality [4]:

$$S_{iklm} B_{lmpq} = \frac{1}{2} \left(\delta_{ip}\delta_{kq} + \delta_{iq}\delta_{kp} \right) . \tag{5}$$

In computer simulations the strain tensor is obtained from two matrices - the **h** matrix describing the system's state (under pressure P) and reference box matrix [5,6] $\mathbf{h}_0$ ($\mathbf{h}_0 \equiv \langle \mathbf{h} \rangle$):

$$'' = \frac{1}{2} \left(\mathbf{h}_0^{-1}.\mathbf{h}.\mathbf{h}.\mathbf{h}_0^{-1} - \mathbf{I} \right) , \tag{6}$$

where $\mathbf{I}$ is the unit matrix of the dimensionality 3. Both $\mathbf{h}$ and $\mathbf{h}_0$ are kept symmetric during simulations. Considering that at equilibrium $\varepsilon_{ij} = 0$, it has been shown [5] that fluctuations of ε_{ij} are related to the elastic compliance tensor S_{ijkl}:

$$S_{ijkl} = \langle \Delta\varepsilon_{ij} \Delta\varepsilon_{kl} \rangle \frac{V_p}{k_B T}, \tag{7}$$

where $\Delta\varepsilon_{ij}$ is the difference between reference and instantaneous states, and the $\langle ... \rangle$ denotes the averaging in the isothermal–isobaric ensemble:

$$\langle f \rangle = \frac{\int d\varepsilon^{(6)} f \exp(-G/k_B T)}{\int d\varepsilon^{(6)} \exp(-G/k_B T)} \tag{8}$$

(for more details see [3,7,8]).

3. $\vec{n}$ and $\vec{m}$ directions

Based on the knowledge of the full tensor of elastic compliances one can calculate the Poisson's ratio for arbitrary direction [9]

$$\nu_{nm} = -\frac{m_i m_j S_{ijkl} n_k n_l}{n_p n_r S_{prst} n_s n_t} , \tag{9}$$

In the equation (9) $\vec{\mathbf{n}}$ and $\vec{\mathbf{m}}$ are unit vectors indicating selected pair of directions (illustrated in the Figure 1) for which the Poisson's ratio is calculated. The $\vec{\mathbf{n}} = (n_x, n_y, n_z)$ vector is oriented in the direction of the applied stress (according to the definition of the Poisson's ratio). The $\vec{\mathbf{m}}$ represents the direction in which the reaction of the system on the applied stress is observed. It is located on the plane orthogonal to $\vec{\mathbf{n}}$, spanned by vectors $\vec{\mathbf{m}}_1$ and $\vec{\mathbf{m}}_2$:

$$\hat{\mathbf{m}}_1 = \frac{\hat{\mathbf{k}} \times \hat{\mathbf{n}}}{\sqrt{(\hat{\mathbf{k}} \times \hat{\mathbf{n}}) \cdot (\hat{\mathbf{k}} \times \hat{\mathbf{n}})}} = \frac{1}{\sqrt{n_x^2 + n_y^2}} \left(-n_y, n_x, 0\right), \tag{10}$$

$$\hat{\mathbf{m}}_2 = \hat{\mathbf{n}} \times \hat{\mathbf{m}}_1 = \frac{1}{\sqrt{n_x^2 + n_y^2}} \left(-n_x n_z, -n_y n_z, n_x^2 + n_y^2\right), \tag{11}$$

where $\hat{\mathbf{k}}$ is the versor of the Oz axis. The versor is the unit vector denoted by symbol $\hat{}$. The α angle describes the orientation of $\vec{\mathbf{m}}$ vector on that plane:

$$\vec{\mathbf{m}} = \hat{\mathbf{m}}_1 \cos\alpha + \hat{\mathbf{m}}_2 \sin\alpha \,. \tag{12}$$

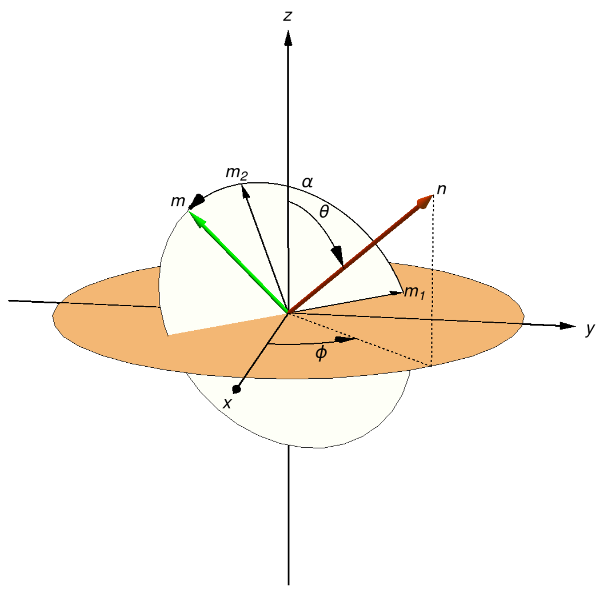

Figure 1. Spherical coordinates: $\vec{\mathbf{n}}$ (described by polar and azimuthal angles θ, ϕ) and $\vec{\mathbf{m}}$ (described by α angle). α is the angle between $\vec{\mathbf{m}}$ and $\hat{\mathbf{m}}_1$ ($\hat{\mathbf{m}}_1$ is the versor created by plane Oxy and plane orthogonal to $\vec{\mathbf{n}}$).

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