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 the 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
- \( \sigma \) – the particles’ diameter
- \( \kappa^{-1} \) – the Debye’s screening length
- \( \epsilon \) – 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
- \( \varepsilon_{ij} \) – component of strain tensor
- \( V_p \) – equilibrium volume of the system
- \( P \) – pressure
- \( p^* \equiv \beta P \sigma^3 \) – reduced pressure
- \( h \) – the box matrix
- \( h_0 \equiv \langle h \rangle \) – the reference box matrix
- \( I \) – identity matrix
- \( \delta_{ij} \) – 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.
- \( v_{an} \) – the Poisson’s ratio
- \( \chi \) – 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]:

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

(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), \( \Delta G \), caused by deformation of a crystal has the form [2]:

\[ \Delta G = \frac{1}{2} V p B_{ijkl} \varepsilon_{ij} \varepsilon_{kl} + ... \]  

(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 constants \( B_{ijkl} \) form the relation between the components of the strain tensor \( \varepsilon_{kl} \) and the stress tensor \( \sigma_{ij} \) [3] (the Hooke’s law):

\[ \Delta \sigma_{ij} = B_{ijkl} \varepsilon_{kl} , \]  

(3)

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

\[ \varepsilon_{ij} = S_{ijkl} \Delta \sigma_{kl} , \]  

(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]:

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

(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] \( h_0 \) (\( h_0 \equiv \langle h \rangle \)):

\[ ^\prime = \frac{1}{2} \left( h_0^{-1} h . h . h_0^{-1} - 1 \right) , \]  

(6)

where \( I \) is the unit matrix of the dimensionality 3. Both \( h \) and \( h_0 \) are kept symmetric during simulations. Considering that at equilibrium \( \varepsilon_{ij} = 0 \), it has been shown [5] that fluctuations of \( \varepsilon_{ij} \) are related to the elastic compliance tensor \( S_{ijkl} \):

\[ S_{ijkl} = \langle \Delta \varepsilon_{ij} \Delta \varepsilon_{kl} \rangle \frac{V_p}{k_B T} , \]  

(7)

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

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

(8)

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

3. \( \mathbf{n} \) and \( \mathbf{m} \) directions

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

\[ \nu_{nm} = \frac{m_i m_j S_{ijkl} n_k n_l}{n_p n_s S_{pqrs} n_p n_s} , \]  

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

\[
\vec{m}_1 = \frac{\hat{k} \times \vec{n}}{\sqrt{(\hat{k} \times \vec{n}) \cdot (\hat{k} \times \vec{n})}} = \frac{1}{\sqrt{n_x^2 + n_y^2}} (-n_y, n_x, 0),
\]

(10)

\[
\vec{m}_2 = \vec{n} \times \vec{m}_1 = \frac{1}{\sqrt{n_x^2 + n_y^2}} (-n_x n_z, -n_y n_z, n_x^2 + n_y^2),
\]

(11)

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

\[
\vec{m} = \vec{m}_1 \cos \alpha + \vec{m}_2 \sin \alpha.
\]

(12)

**Figure 1.** Spherical coordinates: $\vec{n}$ (described by polar and azimuthal angles $\theta, \phi$) and $\vec{m}$ (described by $\alpha$ angle). $\alpha$ is the angle between $\vec{m}$ and $\vec{m}_1$ ($\vec{m}_1$ is the versor created by plane $Oxy$ and plane orthogonal to $\vec{n}$).

**References**


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