CMST 28(3) 81–85 (2022) DOI:10.12921/cmst.2022.0000011

Poisson's Ratio of Yukawa Systems with Nanoinclusions: Nanochannel vs. Nanolayer

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Received: 5 May 2022; revised: 25 June 2022; accepted: 27 June 2022; published online: 9 August 2022

Abstract: The influence of periodically distributed inclusions on elastic properties of crystals in which particles interact through Yukawa potential is discussed briefly. The inclusions in the form of channels oriented along the [001]-direction and layers orthogonal to the [010]-direction are considered. Monte Carlo simulations have shown that, depending on the type of inclusion and the concentration of inclusion particles in Yukawa crystal, qualitative changes in elastic properties occur. In selected directions, one observes appearance of auxetic properties for systems with nanolayers and enhancement of auxeticity for systems with nanochannels.

Key words: negative Poisson's ratio, auxetics, mechanical metamaterials, crystals with nanoinclusions, Monte Carlo simulations, elastic properties of solids

I. Introduction

Colloidal crystals [1] are a relatively new class of materials, whose applications [2, 3] arouse a growing interest among researchers [4, 5]. Some physical properties of charge stabilized colloids can be described by effective interaction potential such as the Hard Core Repulsive Yukawa Potential (HCRYP) [6]. Computer simulations of the face-centered cubic (fcc) Yukawa crystal showed that it exhibits auxeticity [7–10] (i.e. negative Poisson's ratio) in certain crystallographic directions. This effect is observed both for monodisperse crystals [11] and crystals with size polydispersity of particles [12]. Auxeticity of materials has attracted increasing attention of researchers due to their potential applications [13–15]. Recently, a new direction in searching for auxetic materials – models of nanocomposites based on Yukawa crystals – has been proposed [16]. The main idea is the modification of crystalline structure of Yukawa system by introducing into the structure the non-charged colloidal particles which can be viewed as inclusions. The inclusions in the system were arranged in the form of nanochannels or nanolayers [16–18]. The studies showed that by controlling the size of inclusions, as well as their shape and orientation, one can substantially change the elastic properties of the system. One can enhance, weaken or even induce auxetic properties in selected crystallographic directions. In this work the comparison of Poisson's ratios (PR) in selected directions of Yukawa systems with nanochannels and nanolayers is presented.

In the present study, three models of nanocomposites have been considered: two Yukawa crystals with nanochannels (of different sizes) oriented in the [001]-direction and the Yukawa crystal with nanolayer orthogonal to the [010]-direction (see Fig. 1). The considered nanocompos-

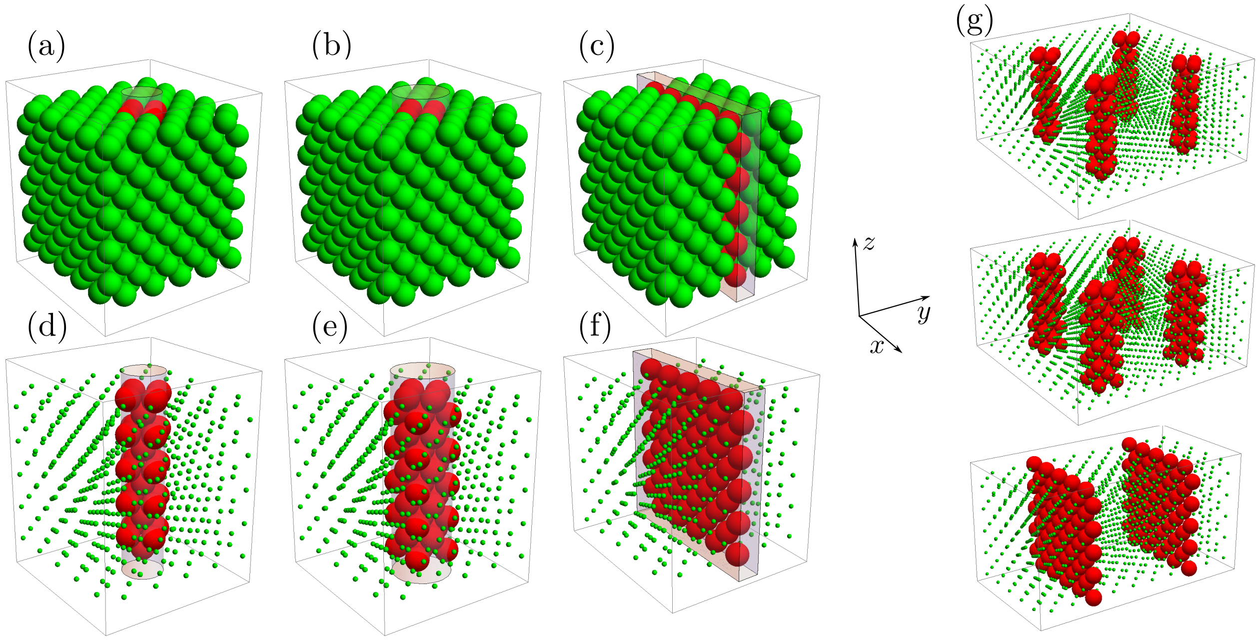

Fig. 1. Examples of studied structures of Yukawa systems with nanoinclusions: (a,d) D-type nanochannel of the diameter $\sqrt{2}\sigma$ oriented in $[001]$-direction, (b,e) S-type nanochannel of the diameter 2σ oriented in $[001]$-direction, (c,f) nanolayer orthogonal to $[010]$-direction, (g) illustration of studied systems in periodic boundary conditions. The particles interacting via Yukawa potential are marked in green colour. Red particles are the inclusion particles. In figures (d–g), the centers of Yukawa particles are marked by green dots to better show the structure of inclusion

ite models are based on the perfect fcc structure. In lattice sites of this structure there are particles interacting via HCRYP [6]:

$$\beta u_{ij}^{\mathrm{HCRYP}} = \begin{cases} \infty, & r_{ij} < \sigma, \\ \beta\varepsilon \frac{\exp[-\kappa\sigma(r_{ij}/\sigma - 1)]}{r_{ij}/\sigma}, & r_{ij} \geq \sigma, \end{cases} \tag{1}$$

where σ is the diameter of the particles' hard core, ϵ is the contact potential, κ is the inverse of the Debye's screening length, $\beta = 1/(k_{\mathrm{B}}T)$, k_{B} is the Boltzmann constant, and T is temperature. Then, as shown in Fig. 1, inclusions in the form of nanochannels or nanolayers have been introduced into the close-packed structure. In the case of nanochannels, their axis has been designated in the $[001]$-direction and for a given diameter of the channel a cylindrical volume containing nanochannel particles has been distinguished. Thus selected Yukawa particles have been replaced by hard spheres (N_{HS}) to model the non-charged colloidal particles. In the case of nanolayer, particles have been similarly replaced for the selected crystallographic plane (010). In the studied cases, the inclusion particles interacted with themselves and with Yukawa particles through hard sphere (HS) potential:

$$\beta u_{ij}^{\mathrm{HS}} = \begin{cases} \infty, & r_{ij} < \sigma, \\ 0, & r_{ij} \geq \sigma. \end{cases} \tag{2}$$

Applying the periodic boundary conditions to thus obtained supercells results in nanocomposite models with a periodic array of nanochannels and nanolayers (see Fig. 1).

II. Simulation Details

The elastic compliances (S_{ijkl}) of considered models have been obtained by Monte Carlo simulations in the isobaric-isothermal ensemble, using the Parrinello-Rahmann method with the variable shape of periodic box [19]. Poisson's ratio for an arbitrary pair of orthogonal directions can be calculated using the formula [20]:

$$\nu_{nm} = -\frac{m_i m_j S_{ijkl} n_k n_l}{n_p n_r S_{prst} n_s n_t}, \tag{3}$$

where n is the direction of the applied stress , m is the direction in which the reaction of the system on the applied stress is observed. The influence of inclusions on PR of studied models has been analyzed with respect to the concentration of hard particles in Yukawa system

$$c = \frac{N_{NS}}{N} \times 100. \tag{4}$$

Computer simulations have been performed for the following dimensionless values of the pressure $P\beta\sigma^3 = 100$, the contact potential $\beta\epsilon = 20$, and the inverse screening length $\kappa\sigma = 10$. The results presented herein relate to systems consisting of $N = 4n^3$ particles, where for the systems with nanochannels $n \in \{4, 5, 6, 7, 8\}$ and for the systems with nanolayers $n \in \{3, 4, 5, 6, 7, 8, 10, 12\}$. The remaining details concerning simulations are the same as in the works [17, 18].

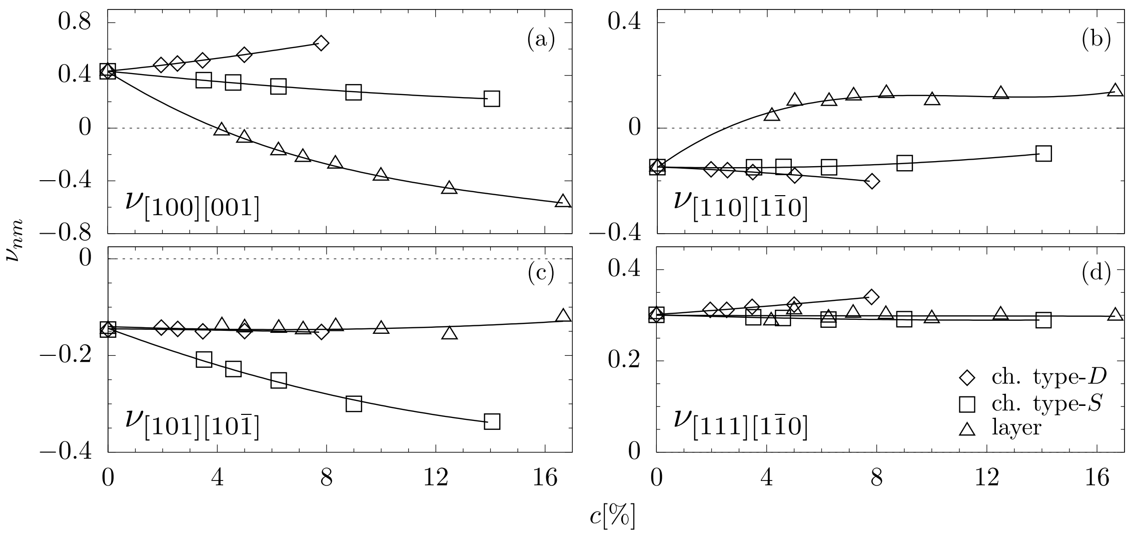

Fig. 2. Dependence of the Poisson's ratio of systems with nanoinclusions on the concentration (Eq. (4)) in the following crystallographic directions: (a) $[100][001]$, (b) $[110][1\bar{1}0]$, (c) $[101][10\bar{1}]$, and (d) $[111][1\bar{1}0]$

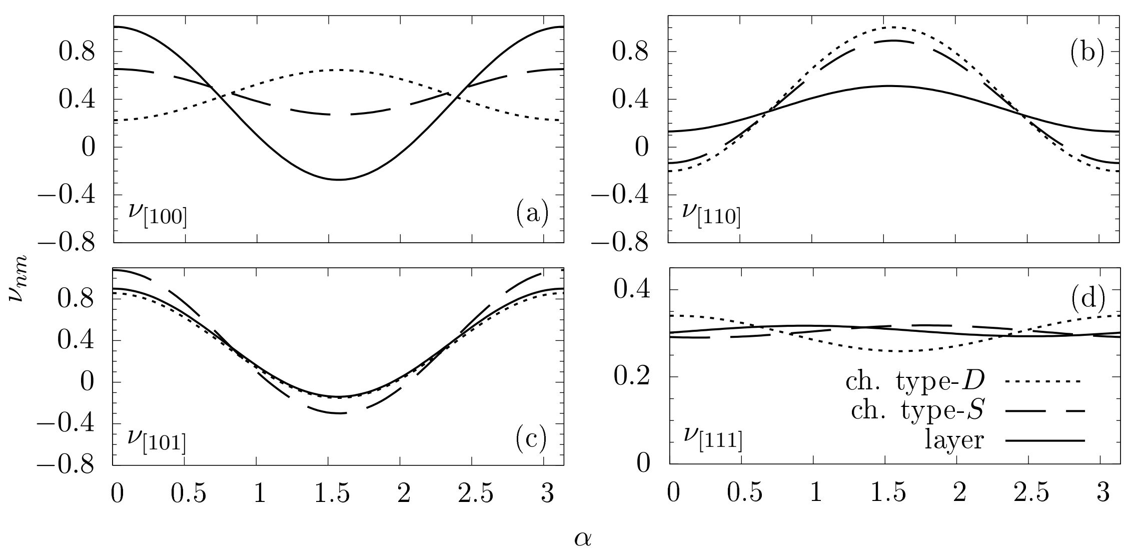

Fig. 3. Dependence of Poisson's ratio of systems with nanoinclusions on the angle α in the following crystallographic directions: (a) [100], (b) [110], (c) [101], and (d) [111]. α is the angle between m and the direction of the line being the cross section of the plane Oxy and the plane orthogonal to n. The concentration of hard particles in Yukawa system with nanochannels of the type D is 7.8% and of the type S is 9%, whereas for the system with nanolayers is 8.3%

III. Discussion

The introduction of inclusions to the system has a significant influence on the Poisson's ratio of crystals in which particles interact with the Yukawa potential. In Fig. 2, the comparison of PR dependence on concentration (c) for studied crystals with nanoinclusions has been presented for four crystallographic directions. The comparison has been made to show that using inclusions of various shapes and concentration one can achieve both qualitative and quantitative changes in the elastic properties of the system and its auxetic properties in particular. The value of Poisson's ratio at $c = 0\%$ corresponds to Yukawa crystal without nanoinclusions. As can be seen in Fig. 2, the introduction of inclusions in the form of nanolayers causes the appearance of auxetic properties in the $[100][001]$-directions (see Fig. 2a) and their disappearance in the $[110][1\bar{1}0]$-directions (see Fig. 2b), while leaving the Poisson's ratio in auxetic direction ($[101][10\bar{1}]$) and non-auxetic direction ($[111][1\bar{1}0]$) almost unaffected (see Fig. 2c and 2d respectively). On the other hand, the introduction of nanochannels of different sizes allows one to enhance auxeticity in $[101][10\bar{1}]$-directions (Fig. 2c) and to weaken it in $[110][1\bar{1}0]$-directions (Fig. 2b). Additionally, such modifications allow one to regulate the Poisson's ratio in a broad range of its positive values in $[100][001]$-directions (Fig. 2a).

Fig. 3 presents the Poisson's ratio of studied systems for any transverse direction to the main crystallographic directions for similar concentrations of hard spheres. Figs. 3a, 3b and 3c show that the Poisson's ratio in the [100], [110], [101]-directions depends strongly on the angle α. Here, the Poisson's ratio changes its value in a broad range from negative to positive ones depending on the type of inclusions. In contrast to that, the Poisson's ratio in the [111]-direction for all systems (Fig. 3d) depends weakly on the transverse direction, which shows low transverse anisotropy of elastic properties of the systems when an infinitisimal load is applied in this direction.

IV. Conclusions

In conclusion, modifications of the crystal structure by introduction of nanochannels allows for a decrease of the Poisson's ratio in $[101][101]$-directions to the value of $-0.34(2)$ [18], whereas the introduction of nanolayers into Yukawa crystal results in appearance of new auxetic directions ($[100][001]$) in which the Poisson's ratio reaches the values down to $-0.57(2)$ [17]. It should be added that in the system without inclusions the latter directions are strongly non-auxetic, with $\nu = 0.43(1)$ [11]. Another interesting result presented in this work is the vanishing of auxetic properties in $[110][1\bar{1}0]$-direction due to introduction of nanolayers into the crystalline structure and it will be published separately.

Acknowledgment

The computations were performed at Poznań Supercomputing and Networking Center (PCSS). This work was supported by grant No. 2017/27/B/ST3/02955 of the National Science Centre, Poland.

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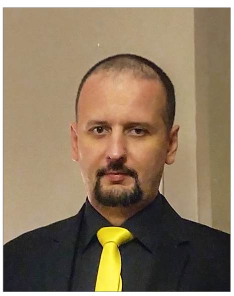

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