Available online at www.sciencedirect.com

ScienceDirect

Procedia Engineering 201 (2017) 543–548

Procedia Engineering

www.elsevier.com/locate/procedia

3rd International Conference "Information Technology and Nanotechnology", ITNT-2017, 25-27 April 2017, Samara, Russia

Elastic constants of colloidal crystals with body-centered cubic lattice and constant potential on the particles

A.A. Batanova[a], P.E. Dyshlovenko[a]*

[a]*Ulyanovsk State Technical University, Department of Applied Mathematics and Informatics 32, Severny Venets Street, Ulyanovsk, 432027, Russia*

Abstract

The model of charge-stabilized colloidal crystals with a monatomic body-centered cubic crystal lattice is proposed to determine elastic constants of the first and the second order. The crystals are described based on the Poisson-Boltzmann nonlinear differential equation. Electric behavior of the colloidal particles obeys the constant potential model. Elastic constants of the crystals are derived from the stress-strain dependencies obtained by means of computational simulation. Elastic constants were obtained for a broad range of lattice parameters. Stability of the crystals and the presence of the many-body effective interactions in them are briefly discussed.

Peer-review under responsibility of the scientific committee of the 3rd International Conference "Information Technology and Nanotechnology".

Keywords: colloidal crystals; Poisson-Boltzmann equation; elastic constants; stress-strain relation; many-body interaction

1. Introduction

The charge stabilized colloidal crystals are spatially ordered systems of electrically charged submicron particles immersed into a liquid electrolyte. They have some technological applications, in particular, in photonic crystal manufacture. They can also serve like models for disordered colloids and more complicated systems of micelles or polyelectrolytes including DNA molecules.

* Corresponding author. Tel.: +7-842-2-778-649.
E-mail address: p.dyshlovenko@mail.ru

1877-7058
Peer-review under responsibility of the scientific committee of the 3rd International Conference "Information Technology and Nanotechnology".
10.1016/j.proeng.2017.09.653

Within the model approach of the present work, colloidal crystals are treated as a medium with initial stress governed by the Poisson-Boltzmann (PB) nonlinear differential equation [1]. The advantage of this approach is that the properties of the system are fully described by solution of the PB equation and no prescribed inter-particle potentials are needed. Owing to the non-zero initial stress, elastic properties of charge-stabilized colloidal crystals have some specificity as compared with conventional crystals [2]. Information about elastic constants is important for specification of the constitutive equations of the crystals.

In the paper, we describe a numerical procedure and carry out computer simulations to obtain stress-strain relations for the crystal with a body-centered cubic (bcc) crystal lattice. Elastic constants of the first and second order are then derived from these relations. Knowing the elastic constants we draw a conclusion about mechanical stability of the crystal. We also detect and estimate the many-body effective interaction in the system.

2. Description of the Model

Colloidal particles in the crystal are charged hard spheres of radius R with constant electric potential φ_0 on the surface. They are spatially ordered and embedded into the binary symmetrical univalent electrolyte (1:1 electrolyte). The centers of the particles are located in the nodes of the bcc crystal lattice with the lattice parameter a (linear size of the corresponding cubic cell).

Electric potential in the crystal obeys the PB equation which, for the case of the 1:1 electrolyte, is

$$\nabla^2\varphi = \frac{2q_e n_0}{\varepsilon_0\varepsilon}\sinh\left(\frac{q_e\varphi}{kT}\right), \tag{1}$$

where n_0 is a bulk concentration of any of two species of the electrolyte, q_e is the elementary charge, ε is a relative dielectric permittivity of the electrolyte, ε_0 is the electric constant, k is the Boltzmann's constant, and T is an absolute temperature. To convert Equation (1) into the dimensionless form, appropriate for numerical solutions, Debye length $\kappa^{-1} = \left(2n_0 q_e^2/\varepsilon_0\varepsilon kT\right)^{-1/2}$ is used for normalising the distances and kT/q_e for normalising the electric potential. Only dimensionless quantities are used hereafter in the paper. Equation (1) takes the following dimensionless form:

$$\nabla^2\varphi = \sinh\varphi\,. \tag{2}$$

Equation (2) incorporates the non-linearity of charge distribution with respect to the electric potential. Hence, the non-linear effects are fully included.

The PB equation is solved within only a single unit cell due to the spatial periodicity of the crystal. The Wigner–Seitz cell of a bcc lattice is used as a domain for the crystal in equilibrium. In the case of non-zero strain, the domain is a deformed initial Wigner-Seitz cell. The interior of the particle is excluded from the domain since the electric potential is just a constant within it. This leads to the following (dimensionless) boundary condition on the particle:

$$\varphi = \varphi_0\,. \tag{3}$$

A set of faces of the domain is resolved into seven pairs of oppositely located faces. The periodic boundary conditions for the electric potential and its gradient are

$$\varphi(\mathbf{r}) = \varphi\left(\mathbf{r} + \mathbf{r}^{(m)}\right), \qquad m = 1, \quad ,7\,, \tag{4a}$$

$$\nabla\varphi(\mathbf{r})\cdot\mathbf{n}^{(m)} = -\nabla\varphi\left(\mathbf{r} + \mathbf{r}^{(m)}\right)\cdot\mathbf{n}'^{(m)}, \qquad m = 1, \quad ,7\,. \tag{4b}$$