Simulation of elastic properties of charge stabilized colloidal crystals

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Charge stabilized colloidal crystals are spatially ordered systems of electrically charged submicron particles immersed into a liquid electrolyte. The particles can vary from simple small plastic balls to complex objects like micelles or DNA molecules. There are a lot of examples of such systems in different fields of technology, chemistry and biology. Recently the interest in them has additionally grown in connection with the creation of self-assembling nanosystems.

While the interactions in colloidal systems can be rather complicated, the electrostatic and entropic interactions are only taken into account in the present study. This allows the use of the mean-field theory leading to the non-linear differential Poisson-Boltzmann equation. The properties of a colloidal system in any particular spatial configuration are then fully determined by the solution of the corresponding boundary value problem. Numerical solution is carried out by the finite element method.

Colloidal crystals are treated here within the approximation of static lattice. Elastic constants are found from the stress-strain and energy-strain dependencies obtained numerically. Charge stabilized colloidal crystals are media with nonzero initial stress. For that reason, description of their elastic properties is a bit more sophisticated than of the conventional crystals. Different approaches to the numerical experiments are discussed.

Elastic constants of different orders are calculated for a number of crystals with monoatomic crystal lattices. Special attention is given to the higher-order elastic constants. In particular, elastic constants up to the fifth order are calculated for the crystal with two-dimensional hexagonal crystal lattice. The results are compared to the graphene data.