Elastic properties of orientationally disordered crystal of mono- and polydisperse hard dumbbells in three dimensions

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Elastic properties of materials are important both for fundamental research and for practical applications. The Poisson's ratio, defined as negative ratio of the change of the transverse strain to the change of the longitudinal strain when an infinitesimal longitudinal stress is applied, is positive for everyday materials, *i.e.* they shrink transversely while being stretched longitudinally. Recently, however, a new group of *materials* has been found, so called *auxetics*, which undergo lateral expansion (contraction) upon longitudinal tension (compression). Thus, auxetics have a *negative* Poisson's ratio. Such materials may find many practical applications and are currently the subject of intensive investigations [1].

Studies of model systems can reveal the influence of various *microscopic* mechanisms on elastic properties and the Poisson's ratio itself. Simulations of simple models interacting through a hard-body potential (infinite when any overlap among cores of particles occurs and zero otherwise) proved that many complex phenomena have purely geometrical origin, *i.e.* they depend almost *exclusively* on molecular shape and size. Monte Carlo simulations of anisotropic hard body systems showed that they are able to mimic various liquid-crystalline and solid phases. In particular, it was shown that a crude model of a diatomic molecule, the hard dumbbell – formed by two fused spheres – beside fluid and fully ordered crystalline phase can form orientationally disordered phase known as rotator phase [2-5]. Its studies allow one to investigate closer the role of molecular anisotropy and orientational disorder on elastic properties.

Elastic properties including the Poisson's ratio of the rotator phase of hard monodisperse dumbbells for various molecular anisotropies were determined by constant pressure Monte Carlo simulations [6]. Simple approximations expressing the influence of molecular anisotropy on the elastic constants and the Poisson's ratio were found. It was observed that the maximum density at which the dumbbells with their mass centers fixed at the lattice sites can freely rotate is strongly correlated with the density at which $C_{12} = C_{44}$. It was also shown that the Poisson's ratio, measured along any direction and averaged with respect to directions transverse to it, is always positive. At any fixed pressure the averaged Poisson's ratio increases with increasing dumbbell anisotropy.

Elastic properties (with emphasis on the Poisson's ratio) of even more disordered system – hard dumbbell rotator phase with polydispersity of `atomic' sizes – are currently under investigations.

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