The Changes of Auxeticity in Hard Sphere Cubic Crystals with Selected Inclusions of Hard Spheres with Different Diameters

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Materials that exhibit negative Poisson's ratio [1], also known by the name *auxetics* [2], are a relatively new class of materials featuring unusual elastic properties. The negative value of Poisson's ratio indicates that when streatched, such material expands its dimensions in at least one of the directions transverse to the direction of the streach. The multitude of potential applications is what drives the interest in auxetic materials. That interest started in the late 1980s, after publishment of an experimental studies by Lakes (who produced the first auxetic foam [3]) and theoretical studies by Wojciechowski (who proposed and rigorously solved the first thermodynamically stable model exhibiting negative Poisson's ratio [4, 5]). These articles constitute an important milestone in the development of auxetic materials. The latter are the subject of intence theoretical and experimental studies. Auxeticity have been found not only in polymers [6] and composites [7], but also in cubic crystals [8]. Alongside the experimental work, a number of theoretical models, showing auxetic properties, have been studied. The most noteworthy (apart from the aforementioned one) are models of rotating rigid units proposed by Grima [9]. Apart from the search for the new materials and models featuring auxeticity and the search for the negative Poisson's ratio in the existing materials, the effort is made to modify the latter to enhance or induce auxetic properties. Thus, recent studies of f.c.c. hard sphere crystals with cylindrical inclusions of other hard spheres with different diameters [10], showed that the partially auxetic behaviour of an f.c.c. hard sphere crystal can be significantly enhanced. This talk will contain the review of further studies performed on the same system, but containing different types of inclusions, which will include quasi 0D (point-like) inclusions, quasi 1D nanochannel inclusions, and quasi 2D layer inclusions (or their different combinations). The investigated systems include (among others) multiple nanochannels oriented in either of the two high symmetry directions ([100] [11] or [111] [12]), as well as models containing inclusions in [110]-directions. The latter is the direction in which auxetic effect is observable in pure cubic systems (without inclusions). It is also shown that the inclusions can be designed such, that the cubic symmetry of the crystal is preserved. An attempt has been also made to verify the impact of inclusions constructed from the simplest (di-atomic) molecules on the elastic properties of the hard sphere crystal. The talk will summarize the changes of elastic properties (with the emphasis on the Poisson's ratio) of the above described models, with respect to the changes of size of particles that form the inclusions, the size of the inclusions them self, and their orientation and layout inside the crystal structure.

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