

Poisson's ratio characterizes deformations of elastic materials. It is defined as a negative ratio of the relative change of the body dimensions in a selected direction perpendicular to the direction of applied load, to the relative change of the body dimensions in the direction of the applied load. For conventional materials its value is positive, e.g. an elastic band becomes thinner when stretched. As many other materials exhibit similar behavior (i.e. values of Poisson's ratio of concrete, glass, aluminum or brass are respectively $0.2 \div 0.37$, $0.29 \div 0.3$, 0.33 , and 0.34) it was long thought that isotropic materials with a negative Poisson's ratio do not exist. Such claims may be found even in respectable textbooks regarding theory of elasticity, e.g., in Landau, Lifshits *Theory of Elasticity*, published in early 90s. Though Almgren presented a mechanical model exhibiting a negative Poisson's ratio in 1985 in *Journal of Elasticity* and shortly after another paper describing thermodynamically stable phase of very simple, hard particles also having a negative Poisson's ratio was published (K. W. Wojciechowski, *Mol. Phys.*, 1987), those examples were treated merely as interesting curiosities. However, once Lakes (*Science*, 1987) fabricated foams and Evans & Caddock (*J. Phys. D*, 1989) manufactured micro-porous materials with negative Poisson's ratio, the interest in such materials is constantly increasing. In 1991 Evans coined term *auxetics* to describe them and this term is used by scientific community ever since. It is worth emphasizing that nowadays auxetic materials constitute one of the important classes of mechanical meta-materials, i.e., systems which unusual properties are determined not by material they are made of but their properly designed internal structure (see J. N. Grima *et al.* *Nature Materials*, 2016).

The main goal of this project is to investigate the influence of small inclusions (typically of the order of few atoms or molecules in at least one direction), periodically placed within crystalline lattice, on elastic properties of selected model crystalline phases with a special emphasis on Poisson's ratio and conditions leading to its negative values. As the size of those inclusions will not exceed few atomic or molecular lengths, at least in one of the dimensions, they will be further referred to as *nano-inclusions*. We plan to investigate systems with crystalline matrices of high symmetry (cubic and hexagonal) and various interactions between the materials of the matrix and the inclusions using computer simulations and analytical methods as well. Preliminary studies of simple atomic and molecular models with infinite inclusions in form of nanochannels and nanowires (K. V. Tretyakov *et al.* *Smart Mater. Struct.*, 2016; J. W. Najroczyk *et al.* *Phys. Status Solidi B*, 2016; P. Piękowski *et al.* *Soft Matter*, 2017) as well as nanolayers and nanoslits (M. Bilski, K. W. Wojciechowski *Phys. Status Solidi B*, 2016; P. Piękowski *et al.* *Phys. Status Solidi-R*, 2016), showed significant influence of these inclusions on Poisson's ratio. In particular, we have shown that introducing nano-inclusions may cause a material to change its Poisson's ratio from positive to negative in certain directions. In aforementioned studies we used analytical methods and Monte Carlo simulations in isothermal-isobaric and canonical ensembles. In parallel, we investigated the influence of *finite*, disjoint nano-inclusions in continuous models using finite element method. Those studies have shown that a negative Poisson's ratio can be obtained not only in already known cases when Young's modulus of inclusions is small comparing to Young modulus of the matrix (which can be considered as an analogue of models of rotating squares) but also when the opposite is true, i.e. when Young's modulus of inclusions is large comparing to Young's modulus of the matrix. Those results can be used to manufacture auxetic materials with Young's modulus much larger comparing to Young's modulus of the matrix.

There are multiple reasons to continue those studies. Fundamental knowledge regarding elastic properties of the systems being within a scope of the project's interest is scarce. The aim of the project is to amend this situation and deliver a wide spectrum of data on that topic. Additionally, such structures can be manufactured experimentally. Thus, having a theoretical insight may inspire many interesting experiments in the near future. It is also worth emphasizing that the currently man-made auxetic materials are porous. In consequence their Young's modulus is low comparing to solid materials which results in their low stiffness severely limiting their practical applications. On the contrary, the materials which will be investigated are all solid and thus our studies may help to manufacture auxetics with large Young's modulus which would significantly boost their utility. Last but not least, those studies will allow to design novel, effective numerical methods for investigation of elastic properties of meta-materials.