A CELL AUTOMATON MODEL OF A TWO-DIMENSIONAL AUXETIC

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A new mechanism is proposed to explain the auxeticity (negative Poisson's ratio) of foams containing stiff grains. The mechanism involves a stochastic migration of stiff grains into cells with soft edges. When a uniaxial compressive stress is applied the migration gives rise to segregation of vacancies toward the lateral surfaces and, as a consequence, to an effective thinning of the sample, as it should be in auxetics. A 2D model based on the cellular automata concept is used to simulate the phenomenon.

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1. Introduction

Auxetics are materials that exhibit unusual mechanical properties. In particular, their transverse dimensions decrease when an uniaxial compressive strain is applied. Strong technological interest is raised about auxetics because of their very high damping properties and of their potential applications. One can cite here personal clothing as crash helmets, body armour or sports clothing, mechanical lungs and sievers, upholstery fabrics with enhanced abrasion properties or biomedical applications as, for instance, applicators for controlled release of drugs. In contrast to ordinary substances such as rubber or glass, auxetics respond differently to the stresses: when pulled they "grow fatter", when pressed they become thinner. This solely feature can be encountered in quite a variety of materials starting from microporous polymers, composites or metals and ending on the single crystal materials. The literature concerning auxetics is vast and increasing in volume [1–6].

Virtually all common materials undergo a transverse contraction when stretched in one direction and a transverse expansion when compressed. The magnitude of this transverse deformation is rendered by a material property known as Poisson's ratio. Poisson's ratio is defined as minus transverse strain divided by the axial strain in the direction of the stretching force. Since ordinary materials contract laterally when stretched and expand laterally when compressed, Poisson's ratio for such materials is positive.

Most auxetics have a microstructure that induces a negative Poisson's ratio at the macroscale, *e.g.* a sort of three-dimensional array made of discrete ribs underlies the negative Poisson's ratio classical auxetic foams [6–11]. Other examples are molecular auxetics, in particular zeolites. It is the organisation of the molecules into a crystal that is responsible here for the type of the microstructure.

2D systems are a very popular choice to study basic properties of materials because of the easiness in their visualisation. As a consequence, they also turn out very helpful in understanding new features. This was, for instance, the situation in the case of granular materials, where 2D models allowed one to understand a number of fundamental phenomena especially at the beginning of the wave of interest. Now the situation repeats in the field of auxetics [12–18].

In this paper we also present a two-dimensional model of an auxetic foam that contains stiff grains. The model is based on the cellular automaton concept. This concept is particularly suitable for the cases when the structure exhibits a certain degree of stochasticity and, at the same time, it consists of a huge number of elements. Auxetic foams are, in principle, heterogeneous. The ribs may have different lengths and widths. The junction angles of the ribs may also vary. If the grains are somehow added to the system, then the overall structure can be very complicated. Also very short and stiff ribs can be understood as stiff grains in our approach.

The paper is organised as follows: in Section 2 a bubble model of the auxetic foam with grains has been introduced. Section 3 describes basic deterministic rules of the automaton. These rules lead to simulation artefacts and had to be improved. In Section 4 we present then refined, more realistic probabilistic rules for the stresses. Finally, Section 5 reports on the resulting histograms of the density and of the thickness of the sample under a uniaxial compressive stress. Section 6 contains a summary and discussion.

2. A bubble model of the auxetic foam

We construct our model as a net of adjacent triangles as shown in Fig. 1. Each triangle forms a cell. The cell can be assumed empty or inhabited by a counter, by which we understand a small and stiff object that can migrate into an empty cell in the surrounding area.

In reality, the counters can be as well short and thick ribs as, also, silica particles in a mixture of silica and polyurethane foam. In view of the recent developments in the design of nanotechnological surfaces it seems

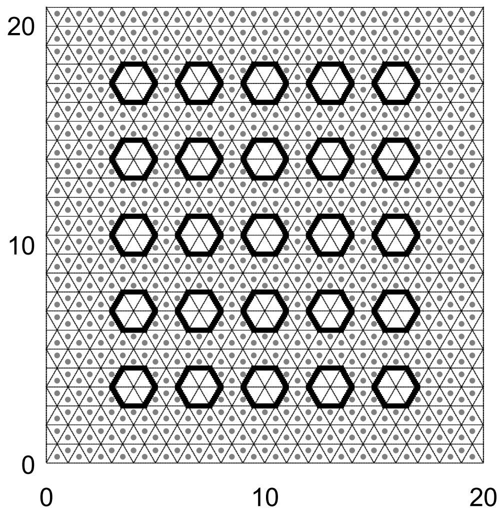

Fig. 1. The geometry of 2D auxetic. The triangles are the cells of the auxetic and the hexagonal structures correspond to the auxetic bubbles with soft edges. The gray dots denote hard counters which have freedom to migrate under acting of stresses.

quite reasonable to realise such a structure as made of appropriate atoms of semiconductors. In such a case the charges travelling at distances much longer than the size of the atoms might play the role of the counters. This is not an entirely new idea. Auxetic properties are already known to arise from the electronic structure of substances, where a negative Poisson's ratio results from an interplay of the occupied and empty electronic states [19].

In two-dimensional system considered in our simulations there exist hexagonal bubbles, whose cells are empty. They are built of six triangular cells, but can be tailored of any shape and size. The bubble cells have soft edges, so under an appropriate stress a counter can enter the bubble through such an edge and remains there as long as no neighbouring cell becomes empty again. This situation corresponds to real mechanisms, although one should bear in mind that the molecular interactions, which lead to such effects, are not known.

The softness of the bubble edges can be larger than that of the surrounding cells. In our case, however, we have assumed the same rules of migrations as well for the bubbles as for the other cells from the volume area. We have also assumed (see Fig. 1) that the system is densely packed with counters and the only empty cells in the initial configurations are the ones belonging to the bubbles.

Two physical properties will be studied in our analysis — the thickness of the sample and the density of the counters. The density is represented by the total number of the counters in a given row and the thickness is calculated as the difference of the column numbers x_{end} and x_{begin}. These numbers are defined as follows. While analysing the states of the cells in a row from the left side to the right side, the first cell encountered, which is not empty, is used to assign the number for x_{begin}. By analogy, the last cell on the right, which is not empty is used for x_{end}. One can describe the state of the sample by monitoring these two properties.

Although our model utilises a honeycomb bubble, it differs from the models, which are usually called honeycomb models. These models are based on the net structure made of stiff arms joined at the ends in such a way that when stretched, they form a hexagonal pattern. Thus, the unusual stretching properties emerge there from purely mechanical aspects. Auxeticity in our systems, as will be seen more clearly later, is determined by different mechanism, *i.e.* by the migration of the counters and the subsequent change in the excluded volume. The assumed model is very simple and belongs to the class of the so-called toy models. It may, nevertheless, provide very useful information.

3. Deterministic automaton

We start with a purely deterministic model, in which any counter, while sensing an empty cell in its vicinity, has no other possibility as to move into this cell. Because of the triangular geometry, each cell has three neighbouring cells. In a dense packing regime, with which we have started, the situation, where all of them are empty, is impossible. However, two empty neighbouring cells may be encountered from time to time at the later stages of the simulations. In this case we had to assume a condition determining, which cell is to be chosen as a new home cell. We have applied a rule of the random choice with equal probability.

As a next step, we have performed a few trial runs. The obtained results are given in Fig. 2 and Fig. 3. The most surprising effect observed is the fact that the results depend on the ways which we perform the adaptation of the cell states. If, for instance, the adaptation of the cells states is performed row by row from the left side to the right, then, as a result, one observes the thinning of the sample at the right edge (see Fig. 2). This is a simulation artifact. Realizing this fact, however, benefits in revealing the importance of the model of the stress propagation.

Figure 3 is even more illustrative. Here the adaptation of the cells states has been done row by row, but now from the sides to the middle of the sample — one from the left and then from the right side at the same time. As a result a big void is created right in the middle of the auxetic.

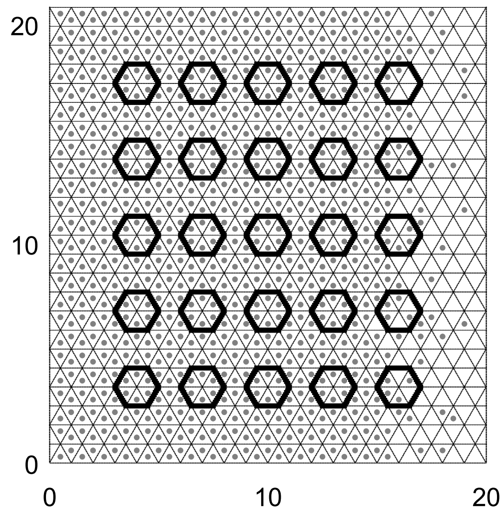

Fig. 2. The configuration obtained when the actualisation of the cells is performed in the row one by one from left to right.

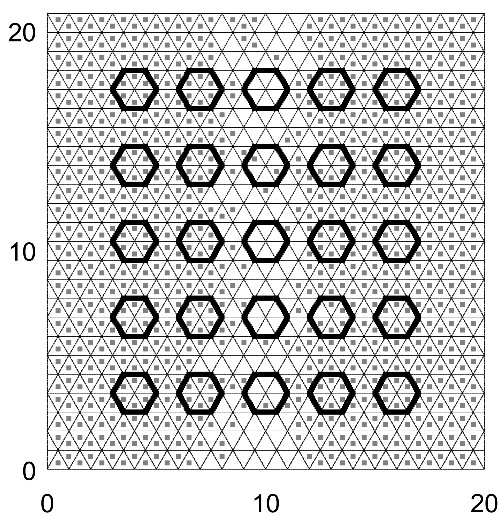

Fig. 3. The configuration obtained when the actualisation of the cells is performed in the row one by one from the left to the middle and from the right to the middle.

The aggregating large voids are interpreted here as simulations artefacts, however such tendency is quite plausible to occur in reality.

One should learn from the present simulations that emptying of the cells takes place toward propagation of the stresses or at the far end from the point where the force is applied. If such a tendency occurred in reality as undesired then the way to avoid it would be, for instance, to tailor the conditions of the pressure application. We can assume nonuniform profile of the pressure or even the profile originating from the set of separate points at which the forces are applied. Studying the subject at the experimental level becomes indispensable here to reveal the real nature of the auxetic systems of this kind.

4. Probabilistic automaton

Bearing in mind that foams are heterogenic and that the tensions within materials propagate on the time scale much smaller than the time scale on which the material structure can respond or rearrange, we have introduced a model in which the adaptation of the cell states within a row is performed by choosing a cell for adaptation at random.

In this case the above discussed artefacts are no longer present and we observe (in Fig. 4) that the sample got thinner at the sides. This effect occurs at the level, where the empty bubbles were present at the beginning of the simulations and is proportional to the number of the large bubbles and to their capability of accepting the stiff grains.

The situation where the voids from the bulk travel toward surfaces can be here compared to the segregation effect in the solids. A real crystalline specimen contains dislocations, grain boundaries and free surfaces. These imperfections are responsible for atomic migrations (diffusion). It is fre-

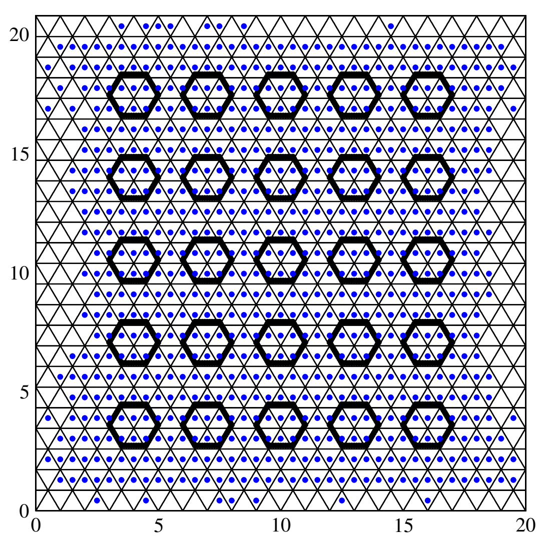

Fig. 4. The configuration obtained when the cell for adaptation within a row is chosen at random.

quently observed that certain elements in a solid solution, initially interspersed homogeneously, as a consequence of diffusion, tend to accumulate at imperfections or segregate to free surfaces. In our case we can interpret then that the voids segregate to a free surface.

5. Larger samples statistics

We consider now a larger system which is built of 600 layers and of 600 columns. In the middle of it there is an area containing $66 \times 70 = 4620$ hexagonal bubbles, which altogether contain 27720 empty cells. The other cells are assumed to be occupied by the counters. The ratio of the empty cells with respect to the total number is 0.077.

The surficial region that is sensitive to pressures consists of 20 layers at the upper part and at the bottom of the sample. The pressure also applies to 20 columns at each side. These numbers, 20 columns and 20 layers, correspond to the condition that we usually applied for the cut-off in the simulations of the Lennard–Jones system, where the cut-off was equal to 20 times the size of the particle. This, however, may seem as a quite thick surface area.

The tension which is applied at the upper and the bottom layers is given by the parameter t. We call cohesion the tension that acts at the sides. It is given by the parameter c. Both parameters take values from the interval [0.0–1.0]. The meaning of these parameters is the following. Because the automaton concept does not use potentials, Hamiltonians *etc.*, one has to introduce these factors in other way. If the resultant pressure is to move a counter from the left to the right, we realize this by adjusting appropriate probability. For instance, if a counter is placed at 10th column at the left side and is subject to the acting of the tension $t = 0.7$, then the probability to move to the right is 70%. We choose a number at random from the interval [0.0–1.0]. If this number is larger than 0.7, then the counter does not move at all, otherwise it goes to the right. If it happens that on the right hand side there are two empty cells, then the counter chooses one of them with the same probability. A similar method of transition probabilities is also used in studying diffusion process in solid solutions [20]. We do not use units in the above rules, but only the dimensionless values of probabilities deciding about the move of a counter from one place to another. However, in reality we know that, for instance, the elasticity of the cell edges would play a role. Then the magnitude of the elastic energy would matter and the above probabilities should be bound to appropriate Boltzmann distributions, analogously to the Monte Carlo simulations.

In next figures, Figs. 5, 6 and 7, we present histograms of the density and thickness of the sample with respect to the Y coordinate, namely to the number of the rows. The first observation is that a narrowing of the sample is observed at the area, where the concentration of the hexagonal bubbles is high. The vertical lines seen in the pictures give the position of this area. The density profiles mirror these dimensions very closely for the early stages of the evolution. However, one observes a widening of the basin area in these profiles, while performing further actualisation of the cell states.

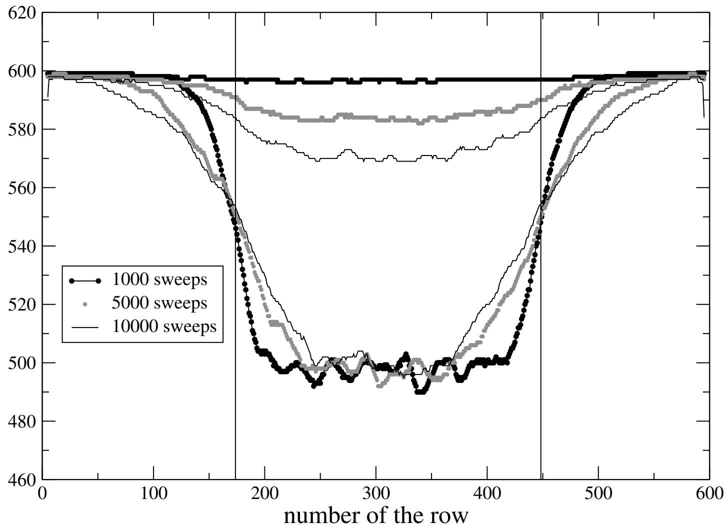

Fig. 5. The profiles of the counters density and the width of the sample obtained for the parameters $t = 0.9$ and $c = 0.9$.

The presented profiles are usually uneven, so to present the tendencies more clearly we use a smoothing averaging over 5 neighbouring states. A sweep here means the actualisation of the cells that consists of the steps whose number is equal to the overall number of the cells in the system.

Because of the acting forces, the hexagonal bubbles gradually fill up with the counters from the neighbourhood. The new empty triangular cells give the possibility of their other neighbours to migrate into them. In this way the counters from the bottom and from the top sides as well as from the edges of the sample can travel toward its middle and the voids, opposite, toward surfaces. In Fig. 8 we show a few examples of the possible trajectories along which a void can travel from the interior of the bubble toward the surface areas.

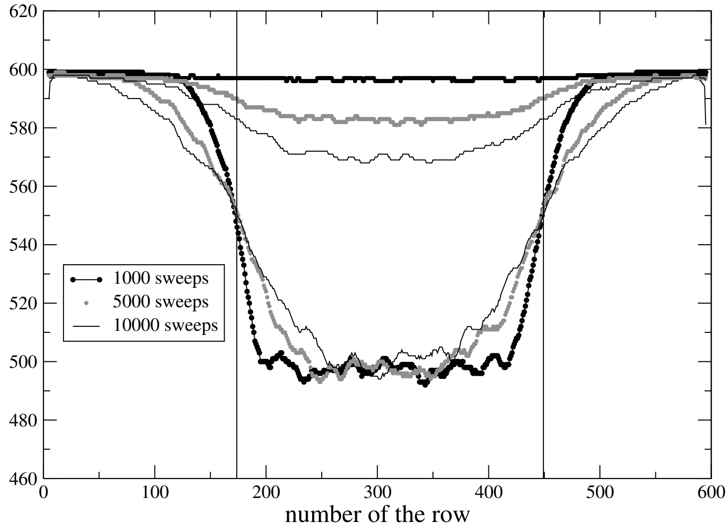

Fig. 6. The profiles of the counters density and the width of the sample obtained for the parameters $t = 0.9$ and $c = 0.5$.

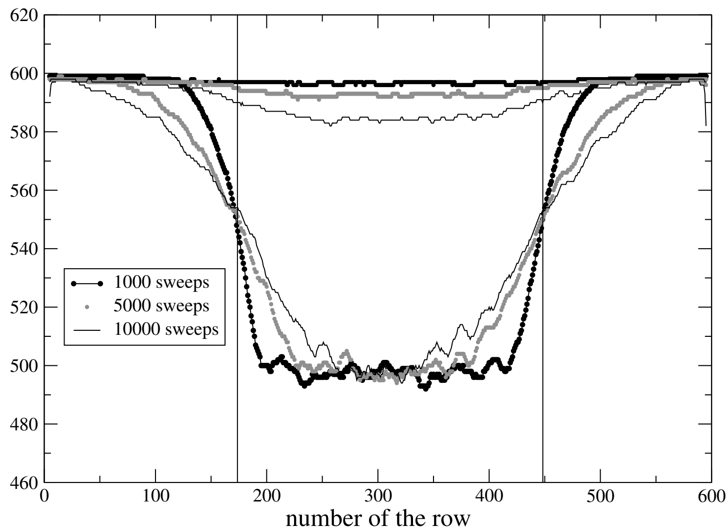

Fig. 7. The profiles of the counters density and the width of the sample obtained for the parameters $t = 0.1$ and $c = 0.9$.

If the tensions equal, then the change in the perpendicular cohesion does not significantly affect the profiles of the thicknesses. This can be seen in Fig. 9, where the solid curve (tension is 0.9 and cohesion 0.09) and the curve with black circles (tension is 0.9 and cohesion 0.5) occur as very similar.

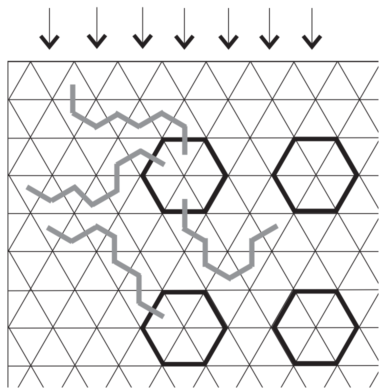

Fig. 8. Examples of the possible trajectories of the voids travelling from the bubble toward the edges. The arrows indicate the action of the external forces.

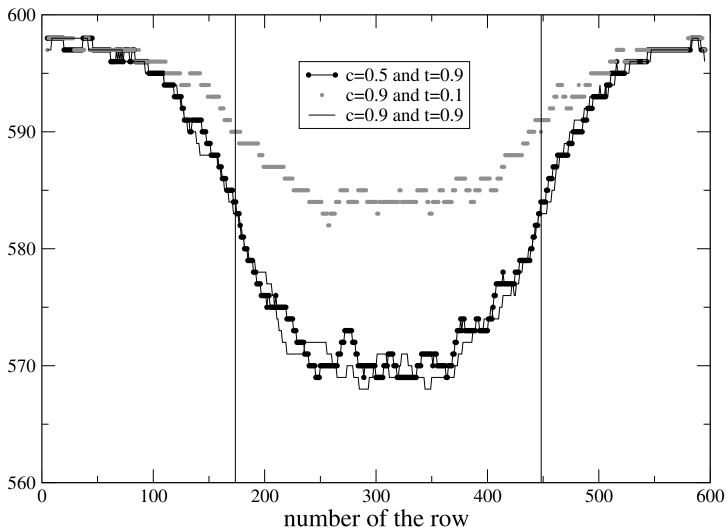

Fig. 9. Comparison of the thickness profiles obtained for the auxetic automaton under different pressures.

6. Summing up

In the above we have presented a simulation model for a two-dimensional auxetic based on the probabilistic tensions. It has been shown that under a uniaxial compression a typical thinning for auxetics is well reproduced. The thinning depends on the number of the bubbles with soft edges into which the stiff grains (counters) can migrate. Such material can be used, for instance, as a sieve. A sketch of it is given in Fig. 10. Under a tension applied at the sides the free spaces occur in the parts made of auxetic material, which in the picture reminds a sausage shape. The free spaces can allow a liquid or a granulate to flow through the sieve. In the case of granulates the size of the spaces determines the size of the grains that can go through the sieve. The dimension of these free spaces will depend on the number and on the architecture of the bubbles with soft edges and can be tailored.

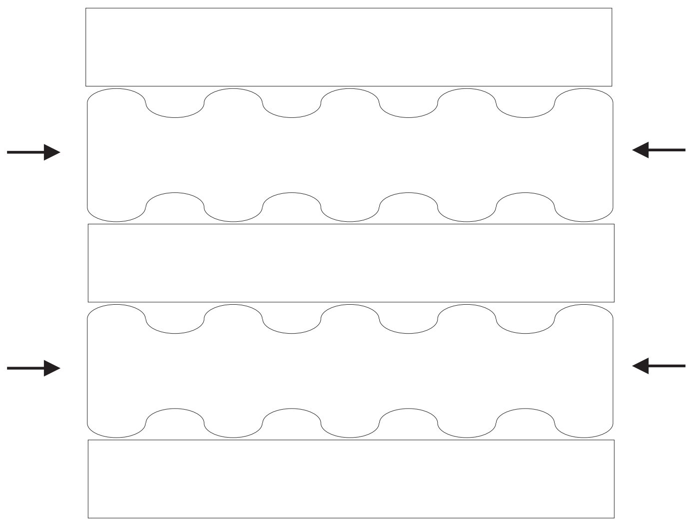

Fig. 10. A possible application of the auxetic as a sieve.

As far as the auxeticity is concerned, one needs to highlight here the major factor that induces the auxetic thinning. This is accessibility of the excluded volume which, when there was no compressive stress, was forbidden to accept particles. This volume, in the present case, relates to the volume of the hexagonal bubbles. Under a stress the elastic soft edges of the bubbles can no longer prevent the counters from going inside. If we imagine that the edges are made of a substance of the rubber type then it will be natural to expect that after releasing the stress these elastic parts would push the counters out of the bubble. Although it seems improbable that upon removal of the stress the sample could regain exactly its initial square shape, the systems of this type can be still legitimately regarded as a kind of non-fully-reversible auxetics.

There is another situation possible: the edges of the hexagonal bubbles are not elastic or, by some other mechanism, the bubbles do not push the counters out. Then, after releasing the tension, the sample remains deformed in the transverse dimension. One can regard this situation as the case of a plastic deformation.

To argue that the reversible changes of the excluded volume are responsible for the auxeticty mechanism we have presented an example that is much more illustrative. Although it can be regarded more as the geophysical phenomenon, this example shows clearly how the changes of the excluded volume can lead to the auxetic type behaviour even on the macroscopic scale.

In Fig. 11 we present a block whose sides are tilted in such a way that they form a sharp edge at the bottom and, at the same time, the front and the back sides are also tilted. This block is immersed in a system of spheres. Now, if we apply a pressure from the front and from the back sides, the block will go up. Because of the geometry a new volume will be accessible to the spheres. As a result the assembly of spheres may get thinner at the sides. If we release the pressure, the block will go down under gravitational force pushing the spheres aside. As a result the system becomes thicker.

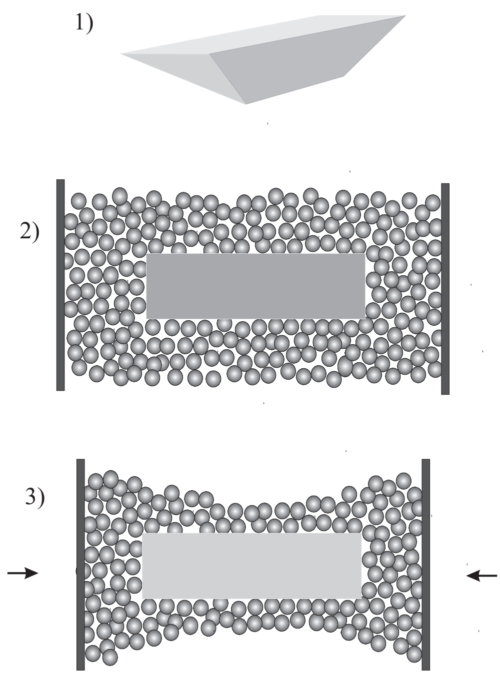

Fig. 11. The effect of auxeticity induced by the pressure on the block immersed in a system of spherical particles. (1) geometry of the block (2) view from above onto the block immersed in the system of the spheres (3) the block is pushed up by the applied pressure and the spheres at the sides enter new space; the system becomes thinner.

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