

PAPER • OPEN ACCESS

Algorithm for foam generation in plane

To cite this article: Olga Klimenkova and Lev Shchur 2021 *J. Phys.: Conf. Ser.* **1740** 012030

View the [article online](#) for updates and enhancements.

You may also like

- [Bonding Yield Analysis of Enclosed Structures](#)
Jakob Visker, Giuseppe Fiorentino and Lan Peng
- [Combinatorial docking approach for structure prediction of large proteins and multi-molecular assemblies](#)
Yuval Inbar, Hadar Benyamini, Ruth Nussinov et al.
- [Study of dimensional changes during washing process for 1:1 interlock cotton yarns](#)
M Szabo, R M Babanatis-Merce, I Barbu et al.



The Electrochemical Society
Advancing solid state & electrochemical science & technology

242nd ECS Meeting

Oct 9 – 13, 2022 • Atlanta, GA, US

Abstract submission deadline: **April 8, 2022**

Connect. Engage. Champion. Empower. Accelerate.

MOVE SCIENCE FORWARD



Submit your abstract



Algorithm for foam generation in plane

Olga Klimenkova and Lev Shchur

Landau Institute for Theoretical Physics, 142432 Chernogolovka, Russia
National Research University Higher School of Economics, 101000 Moscow, Russia

E-mail: oklimenkova@hse.ru, lev.shchur@gmail.com

Abstract. We propose a novel algorithm for the construction of the sparse, nonetheless the massive and rigid structure. The generated structures possess two significant properties reminiscent of the metallic foams. Firstly, the weight of the structures can be as low as the percent of the bulk one. Secondly, the structures are mechanically rigid. The structures are necessary for the simulation of the physical models of the foam properties.

1. Introduction

Foam structures are attracting the attention of researchers in connection with the development of new materials. One of the potential applications for such materials is developing and optimizing hydrogen storage cells [1]. Among such materials, palladium foam stands out in terms of the quality of the pumping cycle and hydrogen release, which is possibly related to the presence of experimentally discovered ferromagnetic properties of palladium foam [2]. Palladium by itself is not a ferromagnet, and there are indications that its low-dimensional forms may exhibit ferromagnetic behavior [3].

It is interesting studying the magnetic properties of foam structures. In this note, as a preliminary step, we propose a method for generating “foam” structures in a plane with characteristics that resemble experimentally obtained foam structures. The main characteristics of such structures are low density, reaching values in a fraction of a percent of the density of similar continuous structures, and satisfying the second property - the presence of mechanical rigidity.

To illustrate the method, we propose an algorithm for generating a foam structure in a plane. This algorithm cannot be straightforwardly generalized to a three-dimensional case, but the basic ideas remain the same. For the foam element, we use a straight line segment of length l . It is easy to generalize the method to the case when the length of the foam elements is not fixed but obeys some distribution with the mean l . Foam elements are randomly thrown inside a square with a side L until the cluster of elements reaches all four square boundaries. This cluster is selected as the foam structure, and those parts of the elements that go beyond the boundaries of the square and those elements that have only one intersection with the cluster are removed from it. The final structures are characterized by the fact that they have a finite and low density, and secondly, they lie on the sides of the bounding square. Note that generating a structure and removing some of the elements resembles making structures with chemical washing [2].

We choose identification of the density of the generated structures using comparison with the strong mathematical results for the properties of the random lines in the plane [4, 5].



The paper is organized as follows. In section 2, we introduce the algorithm for the foam generation in the plane. In section 3, we describe the way the density identification of generated structures. Discussion in section 4 summarized the results.

2. Algorithm for the foam generation

In this section, we describe in the details the algorithm for the foam generation in a plane.

We fix the box with the box size L . Needles of the size l fall randomly on the box. Two needles are wired at the intersection point. The process stops when the foam grown with the needles become rigid, in other words, when the foam can lie at the boundaries as the whole structure and not fall while applying the gravitational force perpendicular to the box surface. We then consider only those needles which belong to the cluster connecting the boundaries. We cut everything which is out of the box.

The model we describe qualitatively reproduce the procedure used in the real experiments [2, 6] consisting of the foam growth and the washing process removing the short components and weakly connected objects. Moreover, the foam structure is very similar to those geometrical objects extracted algorithmically from the collagen gels [7].

The formal description of the algorithm the following.

- (i) Choose the box size L provided with the coordinate system (x, y) equipped with the angle orientation ϕ .
- (ii) Choose the needle length l or choose the distribution of the needles with an average length of l .
- (iii) Generate random numbers for the position (x_i, y_i) , ϕ_i of the needle in the box, where (x_i, y_i) is the coordinate of the first end of the needle within the box ($0 < x_i, y_i < L$) and needle orientation is $\phi_i \in [0, 2\pi)$.
- (iv) Put the needle on the box. We take into account only part of the needle within the box and cut the rest of the needle.
- (v) Remember the intersection points of the needles.
- (vi) Repeat steps 3,4 and 5 until the paths formed with the needles through the intersections will connect all four sides of the box.
- (vii) Decompose structure on the clusters.
- (viii) Choose the most massive (percolating) cluster, ignoring all others. This last procedure is closely related to the experimental washing of the foam [2]).

We use Hoshen-Kopelman [8] algorithm for the cluster decomposition and analysis of the percolation event [9]. To identify the fact that some cluster connects all the boundaries, we introduce the special needles corresponding to the box boundaries. We call four sides **Master0**, **Master1**, **Master2**, and **Master3**, and assign corresponding flags with the **True** values indicating that they belong to the largest cluster. The structure of the **Cluster** is as follows.

```
struct Cluster
{
    int NumberOfCluster;
    bool IsIntersectMaster0;
    bool IsIntersectMaster1;
    bool IsIntersectMaster2;
    bool IsIntersectMaster3;
    int[] NumbersOfFibersInTheCluster;
}
```

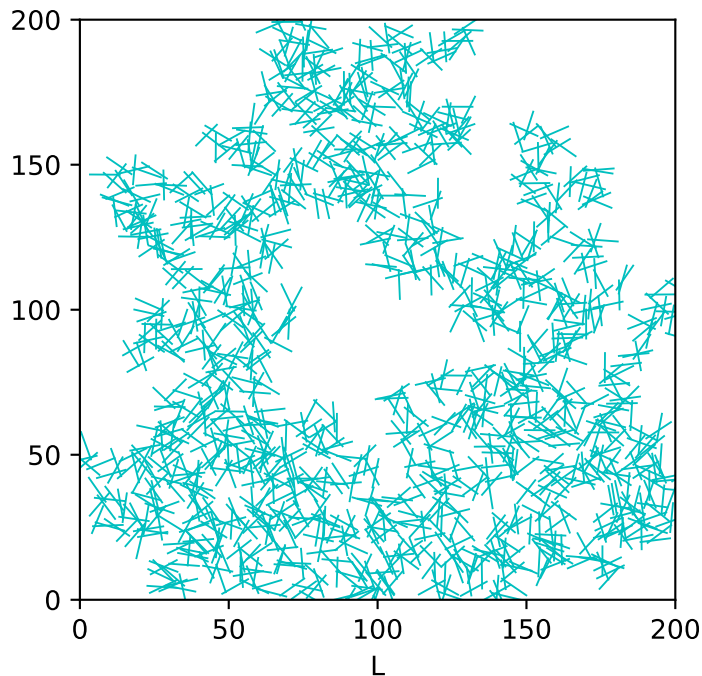


Figure 1. A two-dimensional foam generated in the box $L = 200$ with the needle size $l = 10$.

Example of the two-dimensional foam generated by the algorithm shown in Fig. 1. The foam looks like a very sparse network of connected segments.

Our simulations using the algorithm shows that the rigid washed foam (percolating cluster) can have a density ρ as small as 0.2 for $L = 100$ for the length of the needle $l = 25$ and $\rho = 0.015$ for $L = 500$ for the length of the needle $l = 25$. Asymptotically, for the infinite length of the needle, the density is $\rho = 0.03$ and 0.003 correspondingly. The values are comparable with those obtained for the 3D palladium nanowire foams, which can be as low as $\rho = 0.001$ of the bulk [2].

3. Density identification

The question is, how can one calculate the density of the foam? Our definition of the density relies on the exact results for the random lines in the plane [4, 5].

Miles [4] considered a system of straight lines randomly distributed in a plane and investigated the statistical properties of the polygons formed with the intersected lines. He calculates the mean values for polygons: the mean number of vertices 4, the mean number of perimeter $P = 2\pi/\tau$, and the mean number of area $S = \pi/\tau^2$, where τ is the density. The practical meaning of τ will be identified below.

We use part of the above algorithm to generate structures for comparison, keeping the steps 1-5, dropping the steps 7-8, and changing step 6 with another condition “6a. Repeat steps 3,4 and 5 until the total length of the needles inside the box reached the value l_{tot} ”. We use data structure *Dcel* (doubly-connected edge list) [12] for calculation of the average geometric properties of the polygons formed by the needles. The number of different realization of the foam used for the statistics is $M = 200$.

The simulation was done with parameters: the linear box size $L = 200$, l_{tot} varies from 5000

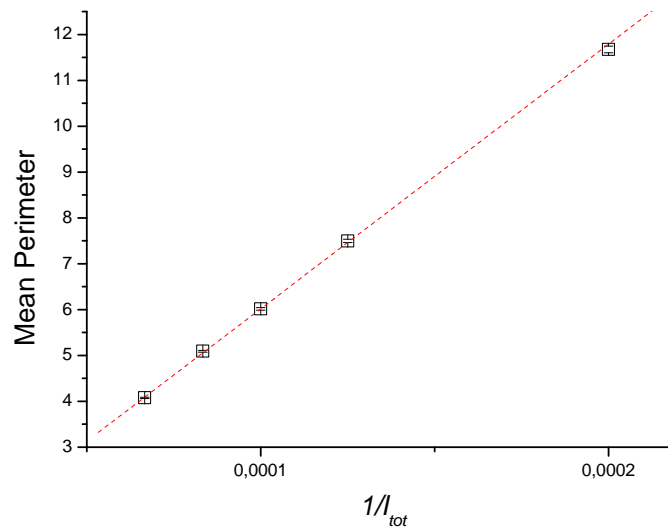


Figure 2. The polygon's mean perimeter as a function of the inverse total length of the needles.

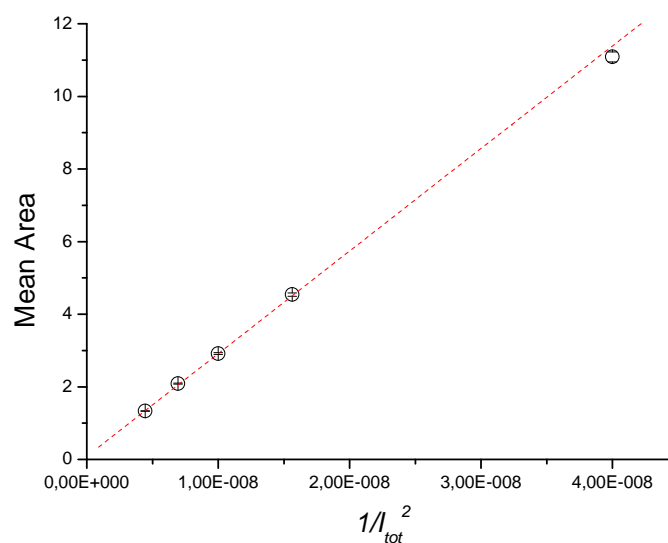


Figure 3. The polygon's mean area as a function of the inverse square of the needle's total length.

to 15000. Figures 2 and 3 show that the mean perimeter and mean area of the polygons formed with the needles behaves inversely proportional to the l_{tot} and the inverse of the square of l_{tot} , correspondingly. Therefore, the density τ introduced by Miles [4] is proportional to the l_{tot} . Properties of the polygons formed by the needles (*the finite objects*) within the box (*the finite objects*) are qualitatively similar to the properties of the polygons formed by the lines (*infinite*

objects) in the plane (*infinite objects*).

Richards [5] developed a procedure to calculate density through the mean number of lines k crossing any straight segment of unit length, i.e., the mean free length of a line. Therefore the mean square of the polygon $S = \pi/\tau^2 = 4/\pi k^2$ and the mean perimeter of the polygon $P = 2\pi/\tau = 4/k$. In simulations, the foam can be covered by the grid with the unit horizontal and vertical spacings. We calculated the number of intersections of the needles with the unit bonds and normalized them by the number of bonds $2L^2$. We use statistics with $M = 200$ samples of foam, and we are able to estimate the value A in $4/k^2 A$, which should be close to $\pi \approx 3.14$ according to Ref. [5]. We obtain numbers in the interval of $A = 3.31 - 3.66$ for the data pictured in Figure 3, and they are close to the π with the accuracy of 5–15 percents. The discrepancy is because our network of the finite needles is not precisely the network of the plane's lines.

Finally, we adopt the procedure mentioned above for the calculation of the foam density.

4. Discussions

We introduce the method for the foam generation and describe in detail the algorithm for the two-dimensional case. The generated structures have two major properties of the real foams, the mechanical rigidity of the structure, and the very small density. We identify the density using comparison with the mathematical results known for the random lines falling in the plane. The resulting structures used in the simulations of the magnetic properties while placing Ising spins on the structure and the results will be published elsewhere [13].

5. Acknowledgments

Discussions with R. Mondaini and R. Scalettar triggers the research. Authors use the HPC facilities of HSE University for simulations. O. Klimenkova is supported by the RFBR grants 20-37-90085 and 20-07-00145. L. Shchur acknowledges the Scientific program of Landau Institute for Theoretical Physics.

References

- [1] E. Antolini, *Energy Environ. Sci.* **2** (2009) 915.
- [2] D.A. Gilbert et al., *Chemistry of Materials* **29** (2017) 9814.
- [3] D.K. Pradhan et al., *Sci. Reports* **9** (2018) 1685.
- [4] R.E. Miles, *PNAS*, **52** (1964) 901.
- [5] P.I. Richards, *PNAS*, **52** (1964), 1160.
- [6] A. Kumar, M.M. Mohammadi, and M.T. Swihart, *Nanoscale*, **11** (2019) 19058.
- [7] A.M. Stein, D.A. Vader, L.M. Jawerth, D.A. Weitz, and L.M. Sander, *J. Microscopy*, **232** (2008) 463.
- [8] J. Hoshen and R. Kopelman, *Phys. Rev. B*, **14** (1976) 8.
- [9] The generated structures are not sensitive to the choice of the random numbers as we check using functions MT19937, MRG32K3A, and LFSR113 from the libraries [10, 11].
- [10] L.Yu. Barash, L.N. Shchur, *Comput. Phys. Commun.*, **182** (2011) 1518; L.Yu. Barash, L.N. Shchur, *Comput. Phys. Commun.*, **184** (2013) 2367.
- [11] M.S. Guskova, L.Yu. Barash, L.N. Shchur, *Comp. Phys. Commun.*, **200** (2016) 402.
- [12] M. de Berg, O. Cheong, M. Van Kreveld, and M. Overmars, *Computational Geometry: Algorithms and Applications*, (Springer, 2008)
- [13] O. Klimenkova, R. Mondaini, R. Scalettar, and L. Shchur, to be published.