Research

Percolation in electrocaloric applications

Švajger Blaž[1,*], Kauskih Pal[2], Kralj Samo[1]

1. University of Maribor, Faculty of Natural Sciences and Mathematics, Department of Physics, Maribor, Slovenia
2. University Centre for Research and Development (URCD), Department of Physics, Chandigarh University, Mohali, Gharuan, India

* Correspondence: Blaž Švajger: blaz.svajger1@gmail.com

Citation: Švajger B, Kauskih P, Kralj S. Percolation in electrocaloric applications. Proceedings of Socratic Lectures. **2026**, 14, 70-74. https://doi.org/10.55295/PSL.14.2026.III6

Abstract:
We study percolation of 3D anisotropic nanoparticles immersed in nematic liquid crystal liquid (NLC). By adjusting the parameters of the simulation, we simulate ordering effects of an external electric field on NLC. We numerically calculate how shapes of particles and the degree of thermal fluctuations impact the percolation threshold. By replacing thermal diodes in an electrocaloric transistor with diodes with nanoparticles close to the threshold we create a self-regulating system which could be exploited in future electro caloric devices.

Keywords: Liquid crystals; Phase transitions; Percolation; Electrocaloric effect

1. Introduction

Percolation theory is a theory that describes the behavior of a network when nodes or links are added (Broadbent & Hammersley, 1957). Nodes and links can be replaced with particles and their connection. This is a geometric type of phase transition, since at a critical number of particles the small, disconnected clusters of particles connect into large, connected spanning clusters. When such clusters connect two sides of a system, we say that the system percolates thus inducing a phase change.

The ElectroCaloric Effect (ECE) is a phenomenon where one triggers reversible temperature changes in a system by adiabatically applying or removing an electric field (Klemenčič et al., 2019). The effect exploits the interplay between thermal (S_{T})) and orientational (S_{O})) contributions to the total entropy $S = S_{\mathrm{T}} + S_{\mathrm{O}}$. In an adiabatic change increased (decreased) alignment of electric dipoles fingerprints in reduced (increased) S_O and consequently in decreased (increased) S_{T}. The latter change is fingerprinted in the temperature change ΔT within the electrocaloric material. An electrocaloric effect transistor is an emerging solid-state thermal management device that utilizes ECE instead of conventional cooling liquids or gases. It controls thermal flux via electrical signals.

In this contribution we show how percolation could be exploited in a representative ECE device.

2. Material and Methods

2.1. Percolation

We illustrate percolation on a simple 2D lattice consisting of squares which are either occupied or emplty. In the initial state all the squares are empty. Then we occupy each of the squares of the system with the probability $p \in [0,1]$ (**Figure 1**) and we perform ensemble averaging. On gradually increasing p starting from $p = 0$ the system becomes percolated at the critical concentartion p_{c}, dubbed percolation threshold. At p_{c} long-range connectivity first appear and the resulting structure exhibits fractal pattern (Mischenko et al., 2006).

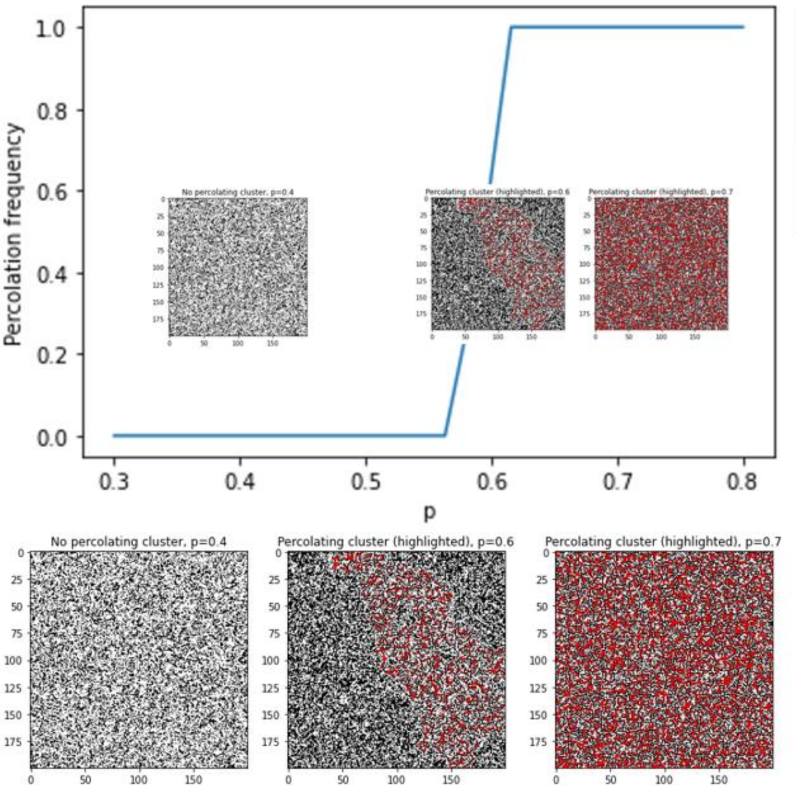

Figure 1. Perocolation of 2D square latice size 200x200. Top: Percolation frequency versus the relative number of active ocupied sites (0-no occupied, 1-all ocupied). Bottom: Three distributions of active sites with red coloured sites marking a cluster that sucessfuly percolates from the bottom to the top of the lattice. Values of p are: left: p = 0.4, middle: p = 0.6, right: p = 0.7.

In our simulation, we consider 3D system of square objects characterised by lengths (a,b,c). We allow them to randomly fluctuate about one axis up the the maximal angle θ_m which we vary in simulation. We study at which concetration of these squares becomes percolated as a function of geometric parameters (a,b,c) and θ_m. To calculate a percolation threshold for given conditions we average results over 100 simulations.

2.2. Electrocaloric effect

The Electrocaloric effect is a phenomenon where applying or removing an electric field ($\boldsymbol{E}$) causes a reversible temperature change under adiabatic conditions (**Figure 2**). This means that the entropy change (ΔS) is zero, therefore any change in entropy because of changing temperature (ΔS_T) must have an equal and opposite change in entropy of order (ΔS_O)(**Figure 3**):

$$\Delta S = \Delta S_T + \Delta S_O = 0. \tag{1}$$

A typical ECE device and its different stages within one cyle (in it the external electric field is switched on and off) is shown in **Figure 4**. Pay attentional to thermal diodes, which control temperature flows to the regions A and B which are in contact with the ECE material. When these diodes are activated, they enable the heat transfer from ECE to the surroundings.

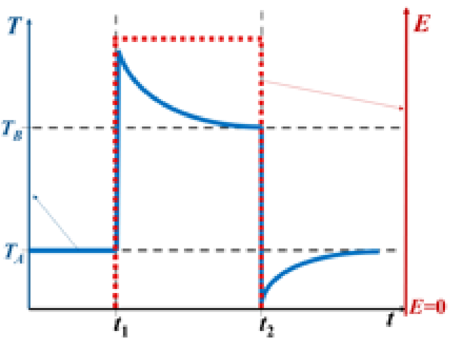

Figure 2. Electrocaloric effect. At t_1 the electric field is activated and the temperature increases from T_A to over T_B. At t_2 the electric field is deactivated and the temperature decreases from T_B to under T_A.

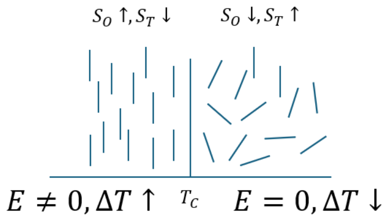

Figure 3. Changing order with electric field ($\boldsymbol{E}$) and the changes in entropy (S_T, S_O) and temperature (ΔT).

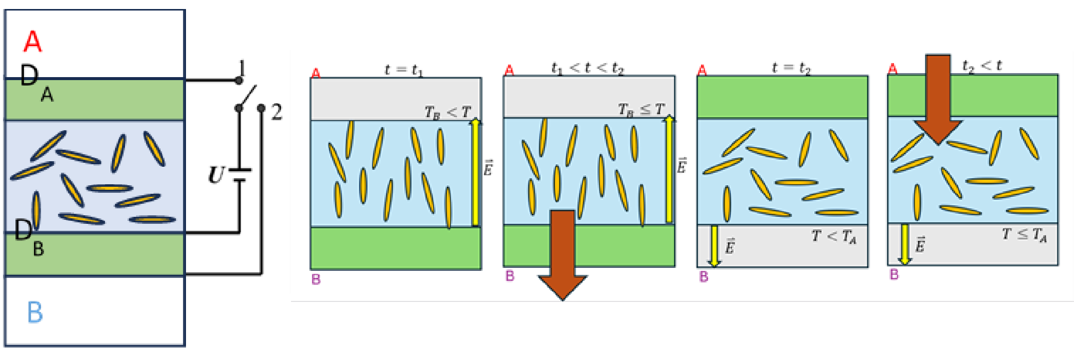

Figure 4. Electrocaloric transistor and phases of it working. A, B are outer materials, D_A, D_B are thermal diodes. The red arrow represents heat transfer, the yellow arrow represents the direction of the electric field. Times coresponds to those in **Figure 2.**

3. Results

Of our interest is to identify geometry of square objects which would exhibit large enough change in percolation threshold p_c on varying θ_m. Here $p = V_n/V_{\text{tot}}$, V_n stands for the total volume of nanoparticles (NPs) and V_{tot} is the total volume of the system. We assume that NPs are immersed in essentially spatially homogeneous nematic liquid crystal (NLC) phase. The degree of its NLC orientational order $\langle P_2^{(NLC)} \rangle$ impacts the degree of orientational order $\overline{P_2^{(NP)}(\hat{e}_i.\hat{n})}$ of anisotropic NPs (van der Schoot et al., 2008). Here P_2 stands for the second order Legendre polynomial, $\langle P_2^{(NLC)} \rangle \in [-0.5,1]$ measures the degree of NLC order, <…> stands for ensemble average, the unit vector $\hat{n}$ determines the average orientation of global NLC order, the unit vector $\hat{e}_i$ describes the long axis orientation of i-t nanoparticle and the overbar $\overline{()}$ indicates the spatial average. $\langle P_2^{(NLC)} \rangle = 1$ fingerprint saturated NLC order where NLC molecules are rigidly aligned along $\hat{n}$. It the case of $\langle P_2^{(NLC)} \rangle = 0$ NLC order is melted into ordinary liquid (the so called isotropic) phase. In our simple model we mimic the impact of $\langle P_2^{(NLC)} \rangle$ on $\overline{P_2^{(NP)}}$ by θ_m. Therefore, larger values of θ_m fingerprint lower order of $\langle P_2^{(NLC)} \rangle$ and consequently lower degree of NPs global degree of order $\overline{P_2^{(NP)}}$. One can tune degree of NLC order by an exteral electric field $\vec{\boldsymbol{E}}$ (Kleman & Lavrentovich, 2003). Therefore, in our simulation different values of θ_m correspond to larger values of E.

In our simulations we systematically explored the impact of NPs geometry and θ_m on the percolation threshold p_c. We identified three geometrires, described in Table 1, that exhibit large enough change of p_c on varying θ_m to be useful in practical applications. The simulation results are shown in **Figure 5**. Geometries of NPs are shown in the left panel of the figure and the corresponding characteristic lengths are given in **Table 1**. One sees that for "shape 2" the percolation threshold changes for 10% on varying θ_m from zero to 80 degrees. This relatively strong variation in p_c could be exploited in self-tunable thermal diods in a typical ECE setup shown in **Figure 4**.

Table 1. Parameters of inserted objects.

Side Object	a	b	c	c/b	a/c
1	0.06	0.02	0.1	5	0.6
2	0.02	0.02	0.2	10	0.1
3	0.1	0.02	0.15	7.5	2/3 = 0.6667

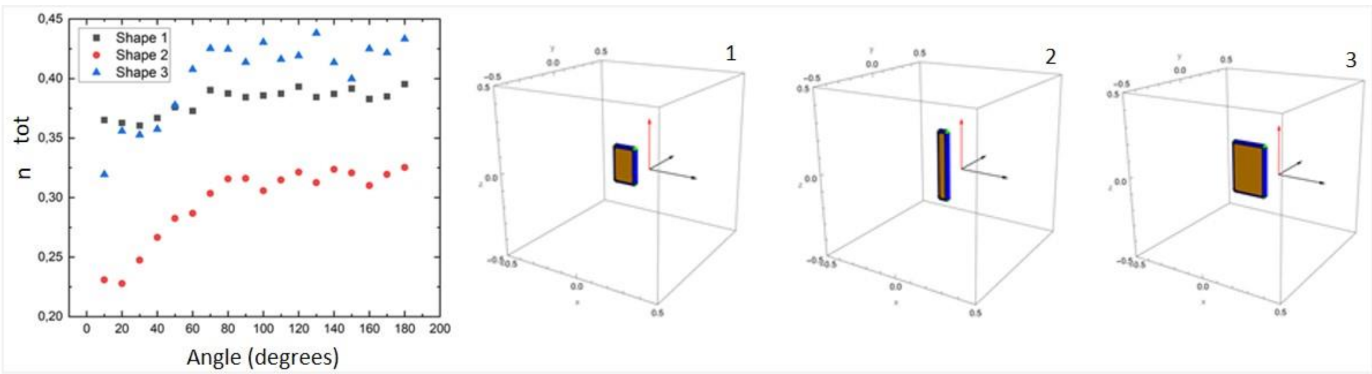

Figure 5. Objects and a graph of their percolation thresholds under different ordering strengths. Left: from top to bottom are shapes 1, 2, and 3 with the red arrow pointing in the direction of the *z*-axis. Right: percolation thresholds (volume of particles/total volume), depending on the permitted angle of deviation.

4. Discussion

The above studied percolation behaviour could be implemented as a self-regulating thermal diode in an ECE device, where a typical set-up is schematically presented in Fig.4. Namely, the thermal diodes in **Figure 4** consist of thermally conduction NPs in NLC matrix. If these NPs are percolated in a desired direction, then large enough heat flow could be established through the diode. This flow could be controlled via an external electric field $\vec{E}$ applied to diodes where a possible set-up is depicted in **Figure 4**. For this reason, the system should be designed as follows. In the absence of $\vec{E}$ fluctuations of NPs long axes should be large enough so that the NPs are percolated. In our simulations this would correspond to relatively large value of θ_m and $p > p_c$ (see **Figure 5**). If the field is applied, then it should switch the system in the nonoperculated regime. Therefore, in our simulations θ_m should be reduced to reach the condition $p < p_c$. Furthermore, one could design a self-regulatory diode which could be tuned to realise a desired temperature in a thermal reservoir. Therefore, if a desired temperature is crossed the diode should switch its thermal conducting state. For this purpose, a desired temperature should reflect in θ_m corresponding to $p = p_c$.

5. Conclusions

In this contribution we briefely described percolation theory and the electrocaloric effect. We described how we simulated percolation in a 3D system and presented the results of our simulation finding that the longer and thiner the object is in the direction of percolation the lower the percolaton threshold and greater the effect of order in lowering the percolation threshold. We discused how we can use the results of our simulations of percolation in diodes to control electrocaloric transistors and offered some posible uses as self regulating diodes. Further study in aplying percolation theory on not ony electrocaloric effect but also other phenomena to study critical values and various thresholds may lead to new discoveries or aplications.

Conflicts of Interest: The authors declare no conflict of interest.

References

1. Broadbent SR, Hammersley JM. Percolation processes: I. Crystals and mazes. Mathematical Proceedings of the Cambridge Philosophical Society. 1957; 53:629-641. DOI: 10.1017/S0305004100032680
2. Mischenko AS, Zhang Q, Scott JF, Whatmore RW, Mathur ND. Giant electrocaloric effect in thin-film PbZr(0.95)Ti(0.05)O3. Science. 2006; 311:1270-1271. DOI:10.1126/science.1123811
3. Kleman M, Lavrentovich O.D. Soft Matter Physics: An Introduction. New York: Springer New York, 2003; pp 337–387. DOI: 10.1007/b97416
4. Klemenčič E, Trček M, Kutnjak Z, Kralj S. Giant electrocaloric response in smectic liquid crystals with direct smectic-isotropic transition. Sci Rep. 2019; 9:1721. Doi:10.1038/s41598-019-38604-9
5. van der Schoot P, Popa-Nita V, Kralj S. Alignment of carbon nanotubes in nematic liquid crystals. J Phys Chem B. 2008; 112:4512-4518. DOI:10.1021/jp712173n