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On the inverse problem of the reconstruction of food microstructure from limited statistical information. A study on bread

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ABSTRACT

The possibility to reconstruct food microstructure by limited morphological information has fundamental importance for theoretical and practical applications. We implemented the simulated annealing method proposed by Yeong and Torquato (1998) for reconstructing bread structure through the information contained into the *lineal-path distribution function*, $L(r)$, and *two-point correlation function*, $S_2(r)$. The method enabled the evolution of two-phase random image toward bread structure. When using the information of *lineal-path distribution function*, the generated images well captured the main morphological features of bread, although several deviations still existed. This was in accordance with the significant differences between the original and reconstructed images as measured by *two-point correlation function*. By hybrid reconstruction, based on both correlation functions, a better reconstruction in terms of both number and size of pores was obtained. In the future the use of more several statistical correlation functions could enable further improvement in reconstruction of bread microstructure.

1. Introduction

Heterogeneous materials are ubiquitous both in nature and in synthetic field. They are composed by different materials or phases or also by the same materials existing in different states. Examples are biological tissues, composites, powders, soil, sandstone, alloys, etc. (Lu and Torquato, 1992a; Jiao et al., 2009). However, food may be clearly classified as heterogeneous materials because consisting in different phases such as fat globules, meat elements, fiber, starch granules, sugars, etc.. More specifically, all food may be considered as two-phase random systems characterized from a voids phase (the pores) and a solid phase (solid matrix). Given these assumptions, bread structure is an excellent example of a two-phase random system composed from pores embedded in the crumb which produce the 3D macroscopic structure (i.e. the crumb texture) worldwide appreciated from the consumers. More specifically, it is widely reported that crumb texture governs the sensorial properties of bread (Pyler, 1988; Baardseth et al., 2000; Scanlon and Zghal, 2001). The cellular structure affects several quality indexes such as the volume of loaf (Zghal et al., 1999), its resilience (Ponte and Ovadia, 1996), the texture during the cooking in oven (Kamman, 1970) as well as the color of crumb that is influenced by the degree of fineness and homogeneity of crumb grain (Gonzales-Barron and Butler, 2008). However not only bread may be considered as two-phase random system but also the sausages which are characterized by fat globules embedded into the minced meat. Other examples are cheeses, ice-cream, coffee beans, roasted coffee cake, beef, fruit and vegetables, to name only few. Recently, the importance of understanding of food microstructure and its relationships with the physical, nutritional and sensorial attributes has been proved from several authors (Van Het Hoff et al., 2000; Aguilera, 2005; Datta, 2007; Parada and Aguilera, 2007). The quantitative and qualitative characterization of microstructure is of crucial importance for both scientific and practical applications, indeed it has influence on conductivity, permeability, mechanical and electromagnetic properties, heat and mass transfers, etc. (Lee and Torquato, 1989; Lu and Torquato, 1992a, b; Torquato and Lu, 1993; Russ, 2005; Baniassadi et al., 2012; Li et al., 2012). In the last decade, the interest of researchers on the characterization of microstructure of heterogeneous materials emerged and several morphological descriptors were proposed. Among these, Torquato and co-authors developed a wide series of statistical correlation functions (SCF) able to extract important microstructure information from two-phase random systems (Lu and Torquato, 1992a, 1993; Torquato, 2002; Jiao et al., 2009). An example is given by the *n-point correlation function* $S_n(x_1, x_2, \ldots x_n)$,

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which is the probability to find n points at position $x_1, x_2, \ldots x_n$ all in the same phase of the system (void or solid phase) (Coker and Torquato, 1995) while the *lineal-path distribution function*, $L^i(z)$, indicates the probability that a segment of length z falls completely in the phase i (Torquato, 2002; Singh et al., 2008). $L(z)$ contains important connectedness informations and gives some indications on the stereology of the system. Other correlation functions such as *chord-length distribution function*, $p(z)$, *pore size distribution function*, $P(z)$, *two-point cluster function*, $C_2(x_1, x_2)$, have been developed and validated for several digitized model systems (identical hard disks, identical overlapping disks, periodic rods, Debye overlapping disks, etc.) and for materials such as sandstone, magnetic gels, Boron modified Ti-alloys (Rintoul et al., 1996; Chan and Govindaraju, 2004; Singh et al., 2008). In addition, Derossi et al. (2012, 2013a, 2013b, 2016) used statistical correlation functions to obtain interesting information on the microstructure of bread and dry-sausages. However, it is worth noting that the statistical characterization of food microstructure is not the only issue. The inverse problem of the reconstruction of food microstructure, from limited statistical information, is still a challenge on which only few experiments have been performed. A precise reconstruction, could provide a non-destructive and relatively low-cost method to estimate the macroscopic properties of food. Yeong and Torquato (1998) proposed an approach to reconstruct random media by using a stochastic method, also known as Y-T procedure. By this method, an initial two-phase random system progressively evolves with the aim to make the statistical correlation functions as much as possible close at those of the original image. Studies performed on digitized model systems, clearly proved as the method enables to obtain a good reconstruction of two-phase random systems using the information contained in some statistical correlation functions (Rintoul and Torquato, 1997; Capek et al., 2009; Li et al., 2012; Baniassadi et al., 2012; Gerke et al., 2014). In a recent study, by using the information of the *lineal-path distribution functions* (LPFs), we reported the possibility to reconstruct the salient features of bread microstructure, although the reconstructed images showed some deviations from the reference structure (Derossi et al., 2014).

In this paper we extended these preliminary results by reconstructing bread structure using several statistical correlation functions. More specifically, the aim of this paper was to implement the Y-T method for obtaining a better reconstruction of bread structure by using the information contained into directional *lineal-path distribution function*, $L(r)$, and *two-point correlation function*, $S_2(r)$.

2. Material and methods

2.1. Bread and image acquisition

Bread loaves were purchased locally and manually cut to obtain slices with a thickness of 1 cm. A 2D image was acquired by using a flat scan equipped with a black box to guarantee constant lightness conditions. A resolution of 600 dpi = 0.004233 mm/pixel was used and the image was saved in TIFF format. A square region of interest (ROI) of 400 × 400 pixels was chosen for the reconstruction on the basis of preliminary tests, in which for bigger ROI no differences in terms of $L(r)$ and $S_2(R)$ were observed. Binary images were obtained using Otsu's method (Sezgin and Sankur, 2004) and the functions the "rgb2gray" and "graytresh" availables in the image analysis Toolbox of Matlab R2012b (Mathworks, USA). Also, the *lineal-path distribution function*, $L(r)$ (LPF), in x and y directions, and the *two-point correlation function*, $S_2(r)$, (TPCL) were extracted from the 2D images by using the algorithms previously developed in Matlab (Mathworks, USA) (Derossi et al., 2012). Particularly, LPF in x and y direction were extracted separately and, as single statistical correlation functions, used for the reconstruction procedure, while TPCL were extracted directly in orthogonal directions. Finally, both the statistical correlation functions were extracted from the void phase of bread (i.e. the pores).

2.2. Reconstruction procedure

Let us consider the reconstruction procedure of a general two-phase random system carried out by using the microstructure information provided from a general statistical correlation function, $f(r)$. Also, let us to define the correlation function of the phase j (equal to 1 or 2) of our "reference" systems as $f_0(r)$ and the lineal-path function of the "reconstructed model" system as $f_s(r)$ which will evolve toward $f_0(r)$. Before reconstruction the "reconstructed model" is a two-phase random system having the same porosity fraction of the reference system. Once the $f_s(r)$ is calculated we can define a new variable E as follows:

$$E = \sum_i \beta_i (f_s(r_i) - f_0(r_i))^2 \tag{1}$$

Where E may be considered as the energy in the simulated annealing method, β_i is an arbitrary weight of the function $f(r)$ and r_i is the distance between two points of the system. To allow the digitized model system to evolve toward the reference system we have the aim to minimize the value of E which is a property that decreases when the difference between the two correlation functions reduce. More precisely, once the first value of E_0 is calculated, an interchange of the states of two pixels falling in different phases is performed enabling to preserve the volume fraction of both phases during the reconstruction. Then a new value of energy, E_1, is calculated as well as the difference of energy between the two different states $\Delta E = E_1 - E_0$. The interchange between the two pixels is accepted via Metropolis algorithm:

$$p(\Delta E) = \begin{cases} 1, & \Delta E \le 0 \\ \exp\left(-\Delta E/_T\right), & \Delta E > 0 \end{cases} \tag{2}$$

Where $p(\Delta E)$ is the probability of accepting an interchange, T is the temperature of the system which progressively decreases as a function of the number of reconstruction steps according to a specific cooling schedule. Particularly, the cooling schedule governs the rate of the temperature changes determining how the systems evolve toward the desired state, without fall in the local minimum energy. In our case, after preliminary experiments, the cooling schedule proposed from Gerke et al. (2014) was used:

$$T_{(k)} = \lambda^{(k-1)} * T_0 \tag{3}$$

Where k is the reconstruction step, λ is a value close to unit and T_0 is the initial temperature. Particularly, in our experiments $\lambda = 0.999,999$ and $T_0 = 0.0001$ were used.

Reconstruction procedure was carried out until the value of energy becomes less than a small tolerance or when a large number (~20.000) of consecutive unsuccessful interchanges occurred (equilibrium condition). For instance, by considering the use of the only *lineal-path function* extracted from the void phase both in vertical (LPF90) and horizontal (LPF0) directions, Eq. (1) becomes:

$$E = \sum_q \sum_j \sum_t \left[LPF_s^{(j,t)}(r_i) - LPF_0^{(j,t)}(r_i) \right] \tag{4}$$

Where q is the number of LPFs extracted in different directions, $b_{j,t}$, are the weights of LPFs in each direction and r_i is the length of a segment of 1, 2, 3 … ….i pixels. An algorithm able to carry out the