THE INHOMOGENEITY PHASE DESCRIPTOR AND NON-UNIFORMITY INDEX FOR DIFFERENT BOUNDARY CONDITIONS

D. Frączek[1], R. Piasecki[2], W. Olchawa[2]

[1]*Department of Materials Physics, Opole University of Technology, Katowicka 48, 45-061 Opole, Poland*

[2] *Institute of Physics, University of Opole, Oleska 48, 45-052 Opole, Poland*

The effective properties of multiphase materials depend mainly on physical properties of the phase components. However, essential meaning have also features of their spatial arrangement, called shortly as morphological features. To perform such an analysis we use digitized two-dimensional patterns of size $L \times L$, which represent samples of real materials. Pixels are treated as finite-sized objects 1×1.

In order to obtain a quantitative characteristics for an average inhomogeneity degree we use entropic descriptors *ED* belonging to statistical physics field [R. Piasecki, Microstructure reconstruction using entropic descriptors, Proc. R. Soc. A **467**, 806 (2011); R. Piasecki, W. Olchawa, Speeding up of microstructure reconstruction: I. Application to labyrinth patterns, Modelling Simul. Mater. Sci. Eng. **20**, 055003 (2012)]. The analysis of the spatial arrangement of *i*-th phase component one can perform making use of phase-component separated phase descriptor, $ED_i = (S_{i,\max} - S_i)/\lambda$, where $S_i = k_B \ln \Omega_i$ denotes the Boltzmann entropy and $S_{i,\max} = k_B \ln \Omega_{i,\max}$ means its maximal theoretical value [D. Frączek, R. Piasecki, Decomposable multiphase entropic descriptor, in review, Physica A (2013)]. For convenience, the Boltzmann constant $k_B = 1$ and $\Omega(k)$ is the number of realizations for a current macrostate (AM) defined as a set $\{m_i(\alpha, k)\}$ of sampling cells $k \times k$ occupation numbers, $\alpha = 1, 2,\ldots, \lambda(k)$. Similarly, $\Omega_{i,\max}$ describes the number of realizations for the reference macrostate (RM) that relates to theoretically maximal uniform configuration at a given length scale.

For purposes of comparison, we also apply the relative index of non-uniformity, $NI_i = (\sigma_i^2 - \sigma_{i,\min}^2)/\mu$, inspired by mathematical statistics, where appear variance and the average per cell of their occupation numbers by *i*-th phase for current configuration and its theoretically the most uniform counterpart, respectively.

The valuable kind of quantitative evaluation of objects arrangement is the multiscale analysis that is usually performed with two-point correlation function. This kind of quantitative characteristics can be also used by the *ED* and *NI* methods. It is sufficient to accept a side length k as the unit of scale of distance expressed in pixels. Now, the determination of influence of type of boundary conditions becomes a natural field of investigations.

The commonly used boundary conditions in statistical physics are hard wall conditions (HWC) and periodic boundary conditions (PBC). The former one is computationally effective but for scales k comparable with a pattern size L does not provide appropriate number of samples. In turn, the latter one ensures the same number of data but consumes much of computation time. In addition, for both types of boundary conditions appears a 'cut-off' of the border clusters. This deformation of the clusters causes changes in values of the internal interface. From the viewpoint of modelling of the effective properties of multiphase materials such behaviour is an undesirable. This is a reason why we consider also the reflecting boundary conditions (RBC), which allows for amelioration of the cutting problem.

The influence of the types of boundary conditions mentioned above on the behaviour of ED_i and NI_i for black phase is illustrated by Figures (1a)-(4a) for arbitrarily chosen three-phase synthetic patterns of size 135×135, which represent different morphologies:

(1) regular chess-board with identical squares 15×15 corresponding to white, grey and black phase,
(2) the corresponding random chess-board,
(3) the white matrix, identical grey clusters while the sizes of black clusters are Gaussian distributed,
(4) black and grey phase irregular aggregates in white matrix simulated with cellular automata.

The observed for ED_i the characteristic scales $k_{\max}$, at which the first maximum appears, and its values quantifies so-called statistical dissimilarity between current macrostate (AM) and reference one (RM), which corresponds to maximal local spatial inhomogeneity. Such a situation indicates for small cluster formation since then dominate the sampling cells with high and low occupation numbers by i-th phase. For the HWC and PBC cases the ED_i curves are similar to each other in contrast to the RBC conditions. In the latter case, the $k_{\max}$ values are shifted slightly on right whereas the values of functions ED_i are generally higher. It is worth to notice that there is once more specific feature distinguishing RBC conditions from the others. Namely, the non-zero values of function ED_i at scales comparable with pattern's side length L can attain relatively high values. These differences result from the construction of the RBC conditions.

The qualitatively similar observations can be found for the non-uniformity index NI_i for the most of length scales. This indicates for possibility of exchangeable applying of both methods at scales $k > k_{\max}$, despite of their different origin. The Figures (1b)-(4b) show significant correlation between ED_i and NI_i indicators for all the considered cases. This is an additional evidence for the local equivalency of the two descriptions of morphological features in multi-phase materials.

Figure captions

Figs. 1-4 (a) The black phase indicators *ED_black* (solid lines) and *NI_black* (dashed lines) against the length scale k for different 3-phase pattern of size 135×135 in pixels given in the inset. The lines colours attributed to the boundary conditions are: black for **HWC**=hard wall, blue for **PBC**=periodic and orange for **RBC**=reflecting boundary conditions; **(b)** The correlation between the two black phase indicators with the same correspondence of the symbols colours.

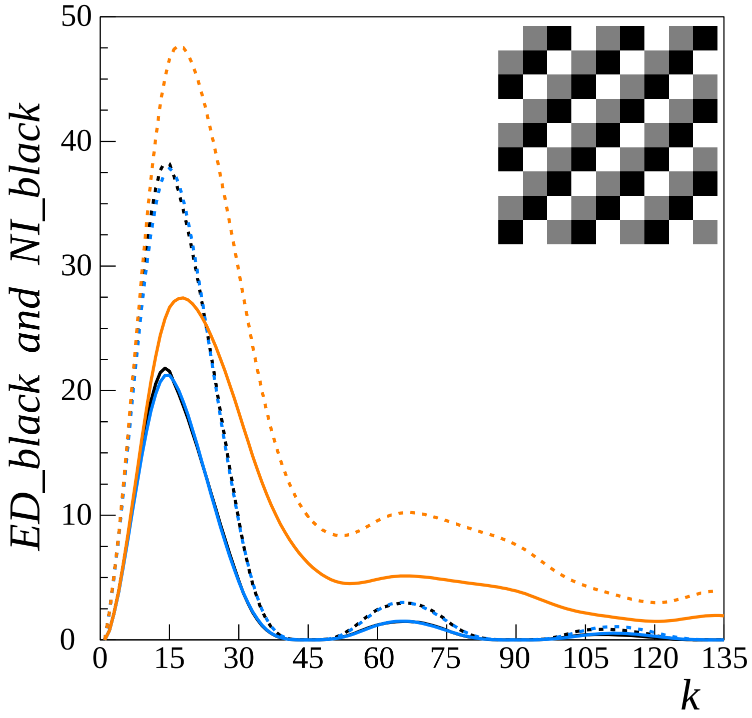

ED_black and NI_black
k
0
10
20
30
40
50
0
15
30
45
60
75
90
105
120
135

Fig. 1a

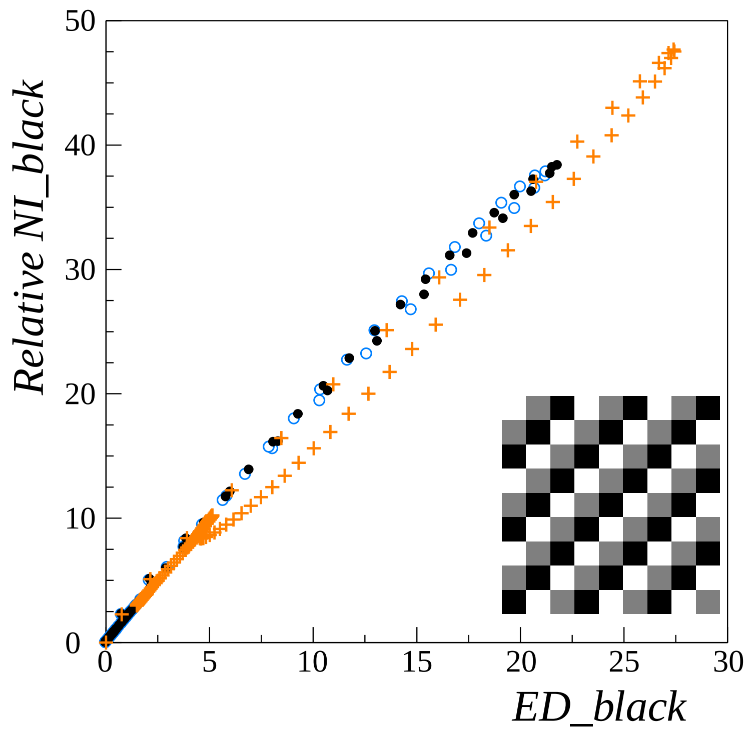

Relative NI_black
ED_black
0
10
20
30
40
50
0
5
10
15
20
25
30

Fig. 1b

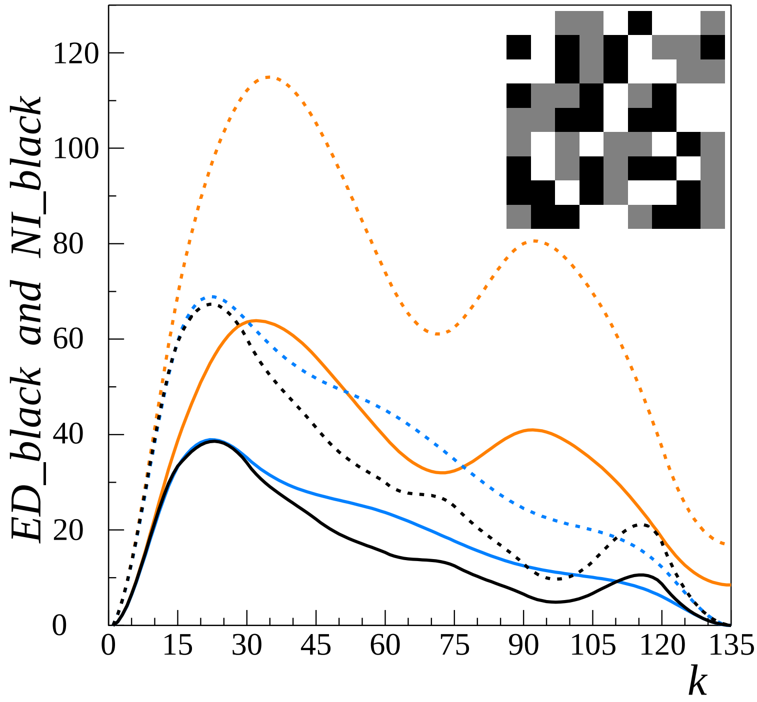

ED_black and NI_black
k
0
20
40
60
80
100
120
0 15 30 45 60 75 90 105 120 135

Fig. 2a

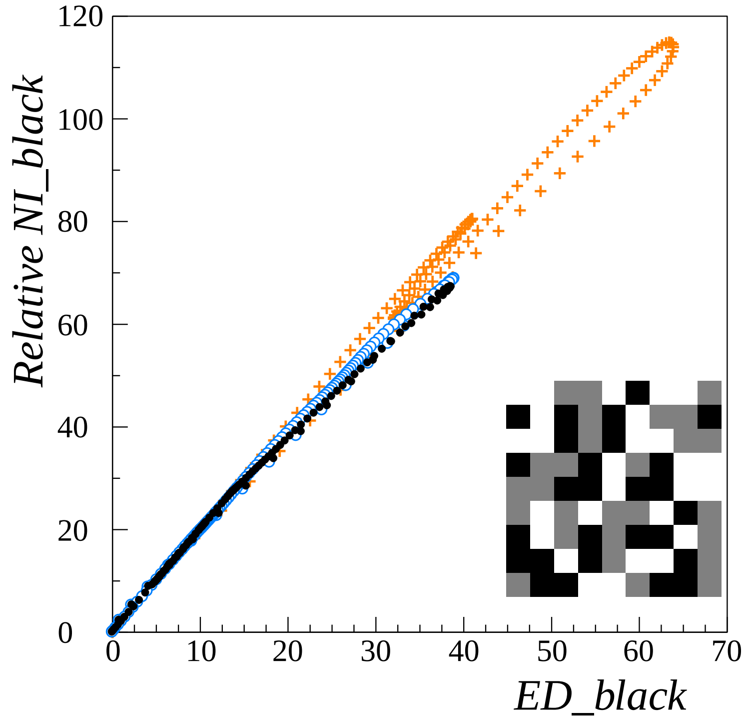
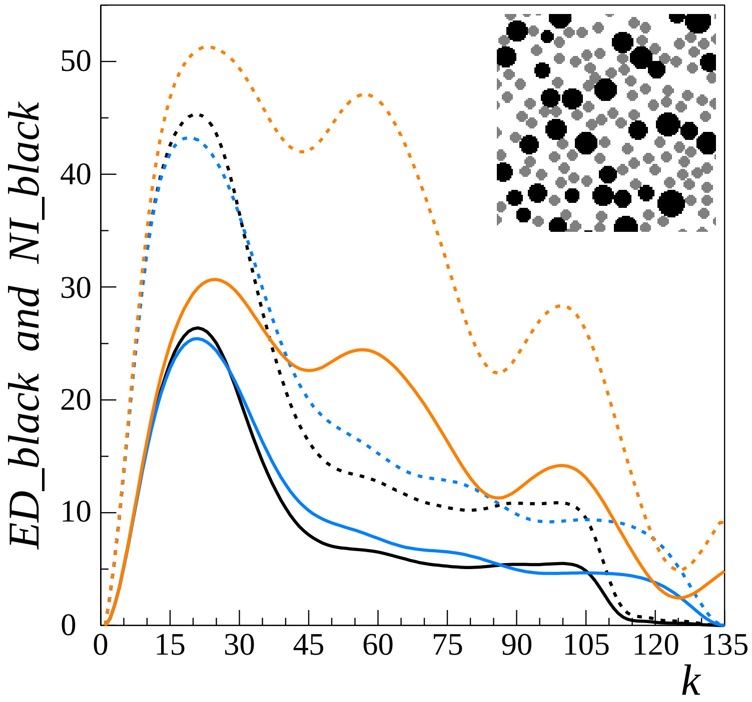
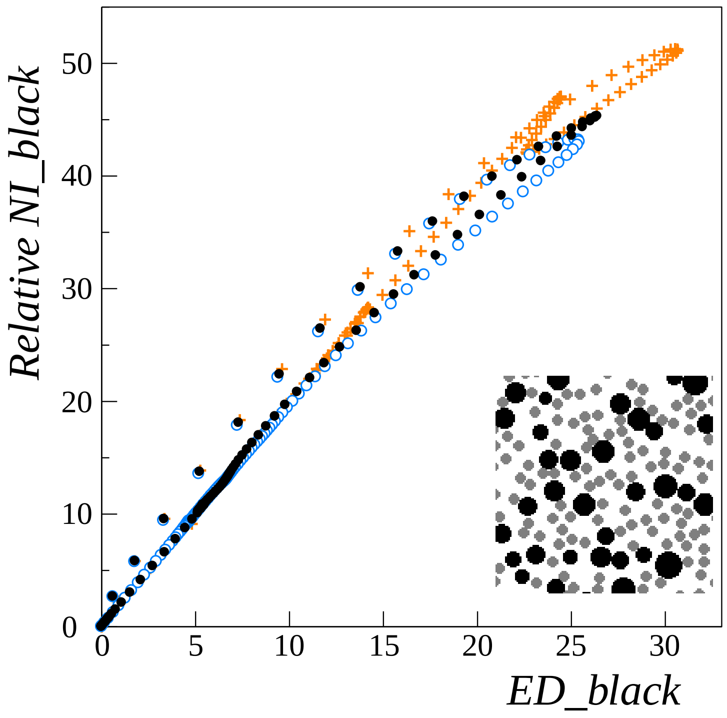

Relative NI_black
ED_black
0
20
40
60
80
100
120
0 10 20 30 40 50 60 70

Fig. 2b



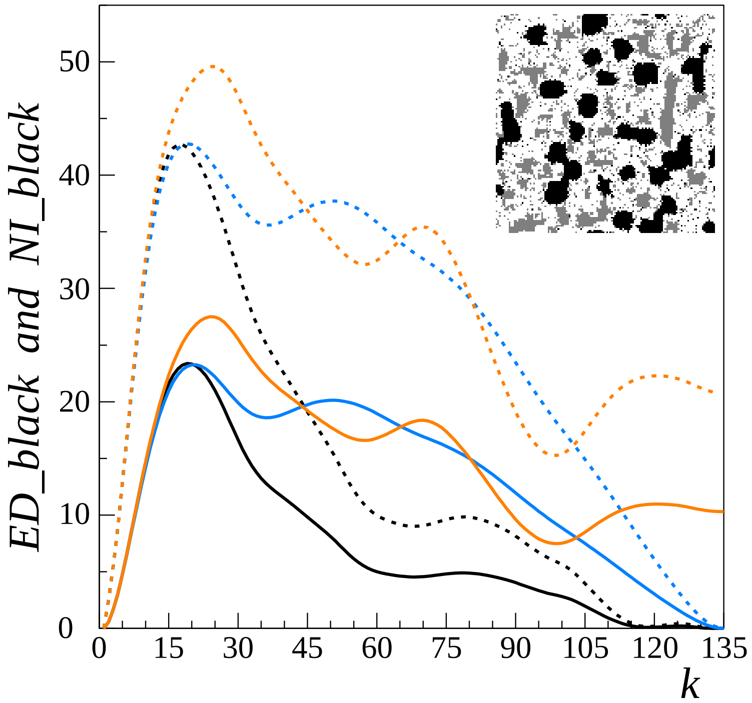
ED_black and NI_black
50
40
30
20
10
0
0
15
30
45
60
75
90
105
120
135
k

Fig. 3a



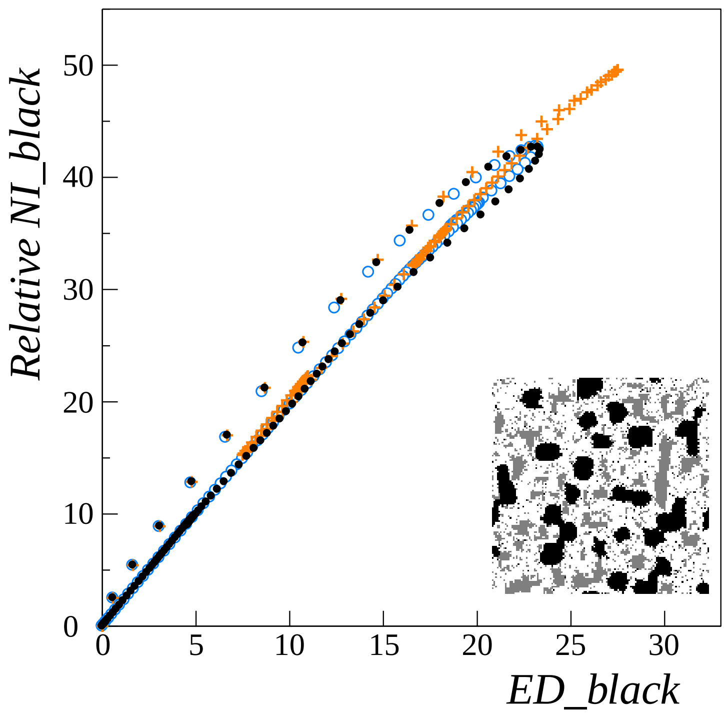
Relative NI_black
50
40
30
20
10
0
0
5
10
15
20
25
30
ED_black

Fig. 3b



ED_black and NI_black
k
0
10
20
30
40
50
0
15
30
45
60
75
90
105
120
135

Fig. 4a



Relative NI_black
ED_black
0
10
20
30
40
50
0
5
10
15
20
25
30

Fig. 4b