Package 'CBAModel'

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Type Package

Title Stochastic 3D Structure Model for Binder-Conductive Additive
Phase

Version 0.0.1.2

License GPL (>= 3.0)

Description Simulation of the stochastic 3D structure model for the nanoporous binder-conductive additive phase in battery cathodes introduced in P. Gräfensteiner, M. Osenberg, A. Hilger, N. Bohn, J. R. Binder, I. Manke, V. Schmidt, M. Neumann (2024) <doi:10.48550/arXiv.2409.11080>. The model is developed for a binder-conductive additive phase of consisting of carbon black, polyvinylidene difluoride binder and graphite particles. For its stochastic 3D modeling, a three-step procedure based on methods from stochastic geometry is used. First, the graphite particles are described by a Boolean model with ellipsoidal grains. Second, the mixture of carbon black and binder is modeled by an excursion set of a Gaussian random field in the complement of the graphite particles. Third, large pore regions within the mixture of carbon black and binder are described by a Boolean model with spherical grains.

RoxygenNote 7.3.2

Imports pracma

NeedsCompilation no

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realize   *Simulate model realization*

Description

Simulates a realization of the stochastic 3D structure model on a 3D grid. The default parameters are those fitted to 3D image data of particular cathode material in Gräfensteiner et al. 2024. For a detailed interpretation of model parameters, we refer to Section 3.1.5.

Usage

```
realize(
  lambdaX = 6.355e-11,
  alpha1 = 205,
  alpha2 = 3944,
  gamma = 1.971,
  mu = 0.499,
  eta = 0.0127,
  lambdaY = 9.34e-09,
  theta = 0.01052632,
  size = 800,
  edge = 150,
  resolution = 20,
  greyscale = c(255, 255),
  progress = FALSE
)
```

Arguments

lambdaX	intensity of the Boolean model mimicking the graphite particles (default: 0.00000000006355 nm^-3).
alpha1	shape parameter of Gamma distribution modeling the length of one semi-axis of the ellipsoidal grain (default: 205 nm).
alpha2	shape parameter of Gamma distribution modeling the length of one semi-axis of the ellipsoidal grain (default: 3944 nm).
gamma	scale parameter of Gamma distribution modeling the length of all semi-axes of the ellipsoidal grain (default: 1.971).
mu	threshold of the excursion set model for the mixture of carbon black and binder (default: 0.499).
eta	parameter of the covariance function of the underlying Gaussian random field. This parameter controls how fine the mixture of carbon black and binder is (default: 0.0127 nm^-1).
lambdaY	intensity of the Boolean model mimicking the large pore regions (default: 0.000000009340 nm^-3).

theta	rate parameter of the Exponential distribution modeling the radii of large pores (default: 0.01052632 nm^-1).
size	the size of the cubic grid, on which the model is simulated (default: 800).
edge	the amount of edge correction used for model simulation (default: 150). The model is realized on a cubic grid, which is extended in each direction by a ceretain number of additional grid points, given by the parameter edge. This avoids edge effects at the boundary.
resolution	the physical distance between to grid points in nm (default: 20). Be careful with changing resolutions, see Figure 5 and the corresponding discussion in Gräfensteiner et al. 2024.
greyscale	this parameter is a 2D vector, which contains the labels for the mixture of carbon black and binder (first entry) and graphite particles (second entry). Note that the pores are always labeled with zero. (default: (255, 255))
progress	Binary parameter. If true, information regarding the progress of the current model realization is printed. (default: FALSE)

Value

Returns a model realization in form of a cubic 3D matrix. The length in each direction is given by the parameter 'size'. At each gridpoint the greyscale value of the corresponding phase is stored. The value 0 indicates pores, while the parameters 'greyscale[1]' and 'greyscale[2]' indicate the carbon black/binder-mixture and the graphite particles, respectively.

References

P. Gräfensteiner, M. Osenberg, A. Hilger, N. Bohn, J. R. Binder, I. Manke, V. Schmidt, M. Neumann (2024) <doi:10.48550/arXiv.2409.11080>

Examples

```
Xi <- realize(size = 10, edge = 10)
```

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