Data in Brief 15 (2017) 840–850

Contents lists available at ScienceDirect

Data in Brief

journal homepage: www.elsevier.com/locate/dib

Data Article

# Programs for the calculation of the spinodal decomposition growth rate and the spinodal gap in nanoparticles

Evgeny Pogorelov [a], Julia Kundin [b,*]

[a] Advanced Ceramics Group, University Bremen, D-28359 Bremen, Germany
[b] ICAMS, Ruhr-University Bochum, D-44801 Bochum, Germany

A R T I C L E I N F O

*Article history:*
Received 23 August 2017
Accepted 17 October 2017
Available online 25 October 2017

A B S T R A C T

This data article contains the programs for the calculation of the spinodal decomposition growth rate and for the modeling of the spinodal gap and concentration profiles in nanoparticles which were used in our article (Pogorelov et al., 2017) [1]. The modeling is based on the mathematical model of spinodal phase decomposition with intercalation rate conditions on the boundaries (Singh et al., 2008) [2].

The maximal growth rate and the parameters of the concentration wave function can be evaluated for a fixed mean composition and intercalation rate. Furthermore, the maximal growth rate as a function of concentration and particle site can be evaluated for various intercalation rates.



**Specifications Table**

| | |
|---|---|
| Subject area | *Physics* |
| More specific subject area | *Spinodal decomposition* |
| Type of data | *Text file* |
| How data was acquired | *Python software, numpy open-source python library* |

DOI of original article: http://dx.doi.org/10.1016/j.commatsci.2017.08.028
* Corresponding author.
*E-mail address:* julia.kundin@ruhr-uni-bochum.de (J. Kundin).

http://dx.doi.org/10.1016/j.dib.2017.10.038

| | |
|---|---|
| Data format | *Python language* |
| Experimental factors | – |
| Experimental features | – |
| Data source location | *Bremen, Germany* |
| Data accessibility | *Data is enclosed to this article* |

**Value of the data**

- The programs are used to analyze of spinodal decomposition in nanoparticles to study the dependence of spinodal gap on the boundary reaction rate and the particle size.
- The codes can be useful for other researchers in the development of further programs for spinodal decomposition in nanoparticles with the intercalation effects.
- The programs are important for the design of stable batteries in energetic technology.

## 1. Data

### *1.1. Program "smax_sp_gap_color.py" for the calculation of the maximal growth rate distribution*

The program is used for the calculation of the maximal growth rate as a function of the concentration, c0, and the particle size, L, for various intercalation rates, R. The maximal growth rate is plotted in a 3D color map. The plot also visualizes the spinodal gap.

```
#########################
# smax_sp_gap_color.py #
#########################
import numpy as np
from scipy.optimize import brentq
import matplotlib.pyplot as plt
from matplotlib import cm
from matplotlib.colors import LinearSegmentedColormap
#To help make good color distribution shifted from default one
def rescaled_colormap(cmap, left, right):
  left=float(left)
  right=float(right)
  cleft=left > 0.
  cright=right < 1.
  if left > =right: return cmap
  if not cleft: left=0.
  if not cright: right=1.
  cdict=(cmap._segmentdata).copy()
  for k, vs in cdict.iteritems():
    v=list(vs)
    if cleft: v.append((left, 0., 0.))
    if cright: v.append((right, 0., 0.))
    v.sort()
    vnew=[]; addpnts=False
    for i in xrange(len(v)):
      if v[i][0]==left:
      if left==0.: vc=v[i][2]
      else: vc=v[i-1][2]+(v[i][0]-v[i-1][0])/(v[i+1][0]-v[i-1][0])*(v[i+1][1]-v[i-1][2])
    v[i]=(left, vc, vc)
    addpnts=True
```