Physica A 412 (2014) 1–18

Contents lists available at ScienceDirect

Physica A

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

Change of scaling and appearance of scale-free size distribution in aggregation kinetics by additive rules

Yuri G. Gordienko *

G.V.Kurdyumov Institute for Metal Physics, National Academy of Sciences of Ukraine, 36 Academician Vernadsky Blvd, Kiev 03680, Ukraine

HIGHLIGHTS

- Aggregation kinetics model by additive rules for 2 cases (pile-ups and walls).
- Scaling laws depend on morphology: diffusive – for pile-ups, linear – for walls.
- Transition between them is caused by the boundary effect.
- Scaling of the cumulative distribution function allows us to find them in experiments.

ARTICLE INFO

Article history:
Received 13 April 2011
Received in revised form 29 March 2013
Available online 25 June 2014

Keywords:
Aggregation kinetics
One-step process
Fokker–Planck equation
Moment analysis
Bootstrapping
Desktop grid

ABSTRACT

The idealized general model of aggregate growth is considered on the basis of the simple additive rules that correspond to a one-step aggregation process. The two idealized cases were analytically investigated and simulated by the Monte Carlo method in the Desktop Grid distributed computing environment to analyze "pile-up" and "wall" cluster distributions in different aggregation scenarios. Several aspects of aggregation kinetics (change of scaling, change of size distribution type, and appearance of scale-free size distribution) driven by the "zero cluster size" boundary condition were determined by the analysis of evolving cumulative distribution functions. The "pile-up" case with a *minimum* active surface (singularity) could imitate piling up aggregations of dislocations, and the case with a *maximum* active surface could imitate arrangements of dislocations in walls. The change of scaling law (for pile-ups and walls) and availability of scale-free distributions (for walls) were analytically shown and confirmed by scaling, fitting, moment, and bootstrapping analyses of simulated probability density and cumulative distribution functions. The initial "singular" *symmetric* distribution of pile-ups evolves by the "infinite" diffusive scaling law and later it is replaced by the other "semi-infinite" diffusive scaling law with *asymmetric* distribution of pile-ups. In contrast, the initial "singular" *symmetric* distributions of walls initially evolve by the diffusive scaling law and later it is replaced by the other ballistic (linear) scaling law with *scale-free* exponential distributions without distinctive peaks. The conclusion was made as to possible applications of such an approach for scaling, fitting, moment, and bootstrapping analyses of distributions in simulated and experimental data.

* Tel.: +380 953890580.
E-mail address: gord@imp.kiev.ua.

http://dx.doi.org/10.1016/j.physa.2014.06.028
0378-4371/

1. Introduction

Many aggregation phenomena in natural processes take place by exchange of solitary agents (monomers) between their aggregates (clusters): phase ordering [1], atom deposition [2], stellar evolution [3], growth and distribution of assets [4], and city population even [5]. In materials science the hierarchical defect substructures that were observed experimentally in deformed metals and alloys appear as a result of some aggregation processes among solitary crystal defects. As a result, the hierarchical defect substructures can demonstrate the self-affine geometry on many scales. In fact, the fractal analysis of fractured surfaces by projective covering and box-counting method shows that the fractured surface can be depicted not only by one fractal dimension, but also by the multifractal spectrum [6–8]. At the same time, surface roughness profiles of periodically deformed Al [9–11], slip line morphology in Cu [12,13], and dislocation patterns in Cu after tensile [14] also demonstrate the self-similar features on many scales. Recently, transition from the homogeneous dislocation arrangement to the scale-invariant structure was described by the statistical model of noise-induced transition [15]. Several other models and theories were proposed to explain the scale-invariant behavior of crystal defect aggregations [16] that possibly lead to the self-affine geometry of fractured surfaces [17].

The general model of aggregate growth on the basis of the simple additive rules that correspond to a one-step aggregation process and its scaling properties are of great interest in this physical context. In such one-step aggregation processes monomers can leave one cluster and attach to another. Usually these exchange processes are described by an exchange rate kernel $K(i,\ j)$, i.e. by the rate of transfer of monomers from a cluster of size i (detaching event) to a cluster of size j (attaching event). Generally, the rate of monomer exchange between two clusters depends on their active interface surfaces that are dependent on their sizes, morphology (line, plane, disk, sphere, fractal, etc.), probability of detaching and attaching events, etc.

Sometimes there is a preferable direction for exchanges, i.e. with asymmetric exchange kernels, $K(i,\ j) \neq K(j, i)$, like in coalescence processes in the Lifshitz–Slyozov–Wagner theory [1], where big clusters "eat" smaller ones. The exchange rate kernel $K(i,\ j)$ is defined by the product of the rate at which a monomer detaches from a cluster of size i and the rate at which this monomer reaches another cluster of size j.

In the Leyvraz–Redner scaling theory of aggregate growth [5] cities A_i of size i evolve according to the following rule:

$$A_i + A_j \xrightarrow{K(i;j)} A_{i-1} + A_{j+1}, \tag{1}$$

where $K(i,\ j)$ is the exchange rate. That is, a monomer (one person) leaves some of the cities A_i of population i and arrives at some of the cities A_j of population j. This can be considered as the generalized rule for the theory of growth and distribution of assets [4], if one can assume that A_i are persons with asset volume of i.

Below, the idealized general model of aggregate growth is proposed on the basis of this approach. The main aim of the work is to use the most profound features of aggregation kinetics and to find the simplest factors that can cause the observed self-affine properties of the aggregating system of solitary agents (monomers) and their aggregates (clusters). In this context, the numerous complex details of the real crystal defect aggregation processes will be hidden behind the idealized and simplified conditions only to emphasize the most general precursors of the scale-invariant behavior of such complex systems.

2. Model

Here detaching and attaching processes are considered *separately* that in the general case could be characterized by different rates. The proposed model significantly differs by this aspect from the other well-known aggregation models in the Leyvraz–Redner scaling theory of aggregate growth [5], the Ben-Naim–Krapivsky theory for exchange driven growth [18], the Lin–Ke theory for migration-driven aggregation [19–21], where detaching and attaching processes are considered *together* in the formalism of the linked Smolukhovski nonlinear equations [22]. Consequently, the different detach product kernel $K_d(n) = k_d S(n)$ and attach product kernel $K_a(n) = k_a S_a(n)$ are taken into account, where k_d and k_a are the measures of activation of detaching and attaching processes, and n is the number of monomers in a cluster. In natural processes k_d is usually determined by the energy barrier for detachment from a cluster and k_a, by the probability for attachment of a migrating monomer to another cluster which is in turn determined by the kind of migration (instant hops from cluster to cluster, ballistic motion, random walking, or their combinations). $S_d(n) = s_d n^{\alpha}$ and $S_a(n) = s_a n^{\beta}$ are the active surfaces of clusters, where α and β are the exponents depending on the morphology of the cluster (for example $\alpha = 1$ for linear clusters and $\alpha = 2/3$ for spherical clusters, and $\alpha = \beta$ in the simplest case of clusters with the same morphology), and s_d and s_a are the constants depending on the morphology of the cluster and the geometry of the neighborhood (for example $s_d = 1$ for linear aggregates and $s_d = \sqrt[3]{36\pi}$ for spherical aggregates, and $s_d = s_a = s$ in the simplest case of clusters with the same morphology and neighborhood). The portion of clusters $f(n, t)$ with n monomers at time t evolves according to the following equation:

$$\frac{\partial f(n,t)}{\partial t} = K_d(n+1)f(n+1,t) + K_a(n-1)f(n-1,t) - K_d(n)f(n,t) - K_a(n)f(n,t). \tag{2}$$