A METHOD OF MECHANICAL CONTROL OF STRUCTURE-PROPERTY RELATIONSHIP IN GRAINS-CONTAINING MATERIAL SYSTEMS*

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Material systems can grow indefinitely large unless there appear some physical restrictions superimposed on them. At first approximation, they can be restricted in their evolution by means of an external mechanical factor such as pressure. If the material system's evolution can be described by a Smoluchowski type equation in the phase space of grain sizes, the average grain size magnitude can be suitably controlled by such mechanical factor. Both magnitude and direction of the factor can render the grain sizes either bigger or smaller than the one expected without any influence of the factor. We propose to embody the mechanical factor in the drift term of the corresponding Smoluchowski equation, in general, derivable from the entropy production principle. Such an embodiment allows one to modify controllably (over certain distinguished time scales of the process) the grain sizes, thus, the mechanically affected material properties such as superplasticity or superconductivity. A simple econophysical example, addressing investment strategies upon random-market tensions, is added to support the overall rationale of the method thus developed.

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1. Introduction

The present paper sketches a method of influencing desired material-structural characteristics of a sample by an external mechanical field, causing a proper embodiment of the resulting material properties during the decisive-stage material formation. The study is based on two types of examples, in addition supported by a related econophysical one.

The first example concerns polycrystalline material formation, addressed in terms of the grain-size Smoluchowski dynamics (SD), assumed that the grains-containing evolution can be terminated at a desired stage with either small or large average grain size. According to an empirical relation, linking the grain size with the corresponding mechanical stress field accumulated over the grain boundaries [1–3], one is able to get a certain termination of the process. After introducing the additional pressure factor, causing to re-distribute the stress field, making then its further propagation improbable, one is able to stop the process at any desired processing instant. Such a control of the process can be achievable by the so-called Hall–Petch–Griffith (HPG) relation [3, 4]. It can yield eventually fine- *vs* coarse-grained polycrystalline materials with different mechanical characteristics — they involve the magnitude of the stress "frozen" within a grain-boundary territory with the magnitude of an average grain's linear size. The size is achievable by the Smoluchowski grain-size phase space dynamics [5, 6], typically close to its stationary Boltzmann-form state (simple HPG relation) or quite apart of that (inverse HPG relation) [3]. In particular, a superplastic material behavior can be obtained by applying so described procedure, such as the one concerning Al-type nanomaterials [1, 2].

The second example, also involves a mechanical pressure-addressing factor, represented by a top-seeded multilayers method of obtaining superconducting YBaCuO ceramic materials. It assumes that one is able to embody to the material the superconductivity property, when a certain secondary phase will be removed from the grain-boundary territory [7]. The experimental strategy relies on squeezing out a molten residual phase this way rendering the grain boundaries clean, *i.e.* devoid of the melt. It results then in improving the material's superconducting properties. In the mentioned multiseeding method, the number of top-seeded layers amplifies the overall effect of squeezing out the undesired molten phase. It has also been utilized in constructing a cuprate's formation model presented by a recent study [8]. The model describes a polycrystalline cuprate's formation within a nucleation-growth phase transition. After the nucleation stage, rich of ripe nuclei of the so-called 123-phase, there remained still an unreacted and molten 211-phase. The ripe nuclei started to evolve, yielding this way a grainy polygonal microstructure, in its flat representation reminiscent of a

Mullins–Von Neumann polycrystalline cellular-network evolution. In order to control the termination of the cellular microstructure, a coarsening procedure has been applied effectively to the network, also benefiting from an escape of the microstructure toward the third Euclidean dimension. For applying the overall cellular network formation, distinguishing between decisive physical time scales responsible for the subprocesses mentioned has become necessary. As a consequence, it led to a microstructure's growth equation formulated in terms of fractional dynamics (FD) [9, 10]. A more closer (than in [8]) look at the dynamics revealed two distinguishable time scales. In what follows, we wish to explore this observation within the context of our method by making use of an address on fractional superconducting domain-growth dynamics, possibly with a Riemann–Liouville integro-differential operator of the order of α [9, 11], pointing specifically to $\alpha = 1/2$, *cf.* [10]. Originally, α has been designated by ω in [8], thus suggesting a crucial involvement of diffusional grain growth, at least in the asymptotic (large times') limit.

Complementing the two above mentioned examples by another, apparently different econophysical one, would, in our opinion, strengthen our overall argumentation on the purposely introduced embodiment of an external mechanically suppressing field. When looking at the dynamics of investments performed by rational traders, we see that a certain opposing, thus tension-making counter-strategy of a group of irrational traders, could be anticipated as a "mechanically" restrictive factor. It causes such traders' dynamics to decelerate or being depressed by the counter-strategy. Qualitatively, such an econophysical microstructural evolution bears a certain similarity to the materials-involving examples.

The paper is structured as follows. In Sec. 2, we would like to present in brief the suitable SD context published in a number of papers [4, 10, 12], in which aggregations in the space of grain sizes have been studied. In the same section, we are going to explain how a typical connection between SD grain growth and stresses' accumulation at polycrystal's overall grain boundaries can be afforded, *cf.* [4] for some preliminary address. In addition, related restricted-market growth example coming out from econophysics has been shown to support our rationale. In Sec. 3, we will make clear the passage between the SD presented in terms of its grain-growth addressing solutions, and the corresponding FD, as has been applied in a preliminary way to cuprate superconductors in [8]. An analogy to the superplastic material counterparts [3] has been introduced in a qualitative way. Section 4 serves to recap the main messages of the paper.

2. Smoluchowski dynamics (SD) and its generic mechanical stress-involving response at stationarity circumstance

Let us begin with the following rationale: there is a phase space $(0, R)$ on which its growth-engaging minimal dynamics is suitably superimposed. R represents the main characteristic linear grain (domain) size, algebraically entailed with the domain volume $(0, v)$ by $v \propto R^d$, rendering the system under study as the one of isotropic (non-tensorial *viz* scalar) character. (d stands for Euclidean space dimension [12].)

2.1. Smoluchowski dynamics with Hall–Petch–Griffith fingerprint

The R-space addressing grain growth dynamics can be expressed as those of Smoluchowski type [13, 14] in isothermal (T = const.) conditions in a following way

$$\frac{\partial}{\partial t}P(R,t) = \frac{\partial}{\partial R}D(R,t)\frac{\partial}{\partial R}P(R,t) + \frac{\partial}{\partial R}\left(\frac{D(R,t)}{k_{\mathrm{B}}T}\frac{d\Phi(R)}{dR}P(R,t)\right), \quad (1)$$

where t is time variable, k_{B} is the Boltzmann's constant. One should bear in mind that the dynamics are presented in the form of a local continuity equation $\partial P(R,t)/\partial t + \partial J(R,t)/\partial R = 0$ with the probability-density ($P(R,t)$) flux, denoted by $J(R,t)$, which is given by

$$J(R,t) = -D(R,t)\frac{\partial}{\partial R}P(R,t) - \frac{D(R,t)}{k_{\mathrm{B}}T}\frac{d\Phi(R)}{dR}P(R,t)\,. \quad (2)$$

The initial condition $P(R,0)$ can be represented by δ-Dirac function [12]. Moreover, the boundary conditions at both ends of the phase space are customarily taken to be reflecting ones. The overall so-stated dynamics help to perceive colloid-matter aggregation phenomena [15] with diffusion and free-energy drift characteristics involved [16]. Notice that such quite peculiar mesoscopic dynamics is acceptable if and only if the diffusion-($D(R,t)$) and drift-($D(R,t)/k_{\mathrm{B}}T$) coefficients are proportional to one another at some constant temperature value of T. Of course, the proportionality goes here without question due to a linearity/proportionality of the diffusion-convection matter fluxes engaged in the system's dynamics [6]. Otherwise, one has to accept a discrepancy from linearity, and a drive toward non-linear Prigogine and Glansdorff (thermo)dynamics enters then unavoidably. At stationarity, one ought to note that

$$\frac{\partial}{\partial t}P(R,t) = 0\,, \quad (3)$$

which is equivalent to infer $J(R,t) = 0$, *cf.* Eq. (2). It implies that practically at $t \to \infty$, one provides

$$P(R) \simeq \exp\left(-[\Phi(R) - \Phi(R_0)]/k_{\mathrm{B}}T\right), \quad (4)$$

wherein the initial value $R_0 = R(t = 0) > 0$. (See [17] for determination of stationary-states in nonequilibrium mesocopic-thermodynamic systems.) Thus, there is one single, physically legitimate energetic (Kramers-type) barrier, $\Delta\Phi(R) = \Phi(R) - \Phi(R_0)$, termed the free growing-system energy barrier. It conforms, if unperturbed, to the drive of the system by means of typically decreasing $\Phi(R)$ course until arriving at an affordable stationary state.

The free-energy ($\Phi(R)$) gradient, substantiating the stochastic force, constitutes the drift function of the SD, $B(R, t)$, which reads at stationarity (as $t \to \infty$) as follows

$$B(R, t \to \infty) = -\frac{d\Phi(R)}{dR} \times \frac{D(R, t \to \infty)}{k_{\mathrm{B}}T}\,, \tag{5}$$

wherein the stochasticity manifests if R came upon to be a stationary stochastic variable [16].

The information about the system, *cf.* Eqs. (1)–(5), has to be concisely recapped as follows:

(i) depending on the type of matter aggregation *vs* agglomeration process, and the physical force-field scale it addresses, the diffusion function $D(R, t)$ (in particular, when applying the scaling law, $v \propto R^d$) can be constructed from the main driving deterministic and stochastic contributions to the aggregation. Thus, it can typically be driven by mass-convection, capillary forces and/or diffusion itself [5, 6];

(ii) based on the same construction line, the free energy $\Phi(R)$ (mainly, within the entropy-producing matter rearrangements), *cf.* Eq. (5), can be derived too [5].

The stationarity condition at $t \to \infty$ comes out to be a challenge here, especially if the mechanical-stress exerting intergrain-boundary fields are (upon late-stage growth) being involved fairly interchangeably [4, 15]. It may, owing to the grain-size magnitude obtained [2, 3], appear either at short-time or late-time regimes. The challenge here means that it should be controlled by the experimental conditions. It implies that one could either stop the growing process at some (relatively) short-time R-value, presumably if $R \sim R_0$, or prolong purposely the termination up to more pronounced time regime in which $R \gg R_0$ occurred.

Such a differentiation addresses then the possibility of embarking either on small-grain size values (short-time interval) or, on the contrary, one should arrive at quite a large-grain size values obtained. The former ($R \sim R_0$) makes an indication of superplastic *viz* fine-grained

(nano)materials [2], whereas the latter ($R \gg R_0$) points to the plastic, and sometimes, depending on the cohesive force-field within the polycrystal, even brittle material samples [4].

At stationarity, which is a fairly time-independent regime, one would be able to address this material *vs* mechanical-strength circumstance in terms of a well-established issue [3]. Such issue appears to be the HPG (soft) material's mechanical-strength relationship, addressing the overall (non)late-stage grain-growth size as compared to the stress (σ_{mech}), accumulated in some respective amount within the material's (inter)grain boundary space [2, 3, 10].

The HPG scaling relation [10], as applied to our type of argumentation scheme, would read as follows

$$\sigma_{\mathrm{mech}}(t_{\mathrm{s}}) \sim \left(\frac{1}{R(t_{\mathrm{s}})}\right)^{\nu_{\mathrm{HPG}}}, \tag{6}$$

wherein $\nu_{\mathrm{HPG}} = 1/2$ holds for typical (*e.g.*, metal polycrystal [2, 3, 18]) grains-containing material [19]; t_{s} would correspond to the characteristic stationarity time, *i.e.* at which time value one is able to arrive at it in a controllable way [1, 4]. If $\nu_{\mathrm{HPG}} \neq 1/2$, one would anticipate some discrepancies from classical HPG relation [10]. There exists, however, a rigorous and quite practical [1, 3] differentiation of material mechanical characteristics based on modification of the HPG relation. Such modification indicates whether the materials after physicochemical, *e.g.* high-pressure involving treatments [1, 20], are structurally fine-grained ($R \sim R_0$) or become rather coarse-grained ($R \gg R_0$). The case of $R \sim R_0$ causes the inverse (or, reverse) HPG relation (iHPG) to apply, *i.e.* if $\nu_{\mathrm{HPG}} < 0$ (see, Fig. 1). The case of $R \gg R_0$, in turn, addresses the nonfine grained microstructure [3, 20]. $\sigma_{\mathrm{mech}}(t_{\mathrm{s}})$ goes like $t^{\nu_{\mathrm{HPG}}}$ according to positive (iHPG) or negative (HPG), *i.e.* in a non-exponential way [4, 10, 15, 18]. As to regulate the stationarity working condition, Eq. (5), appropriately, there exists some high-pressure experimental method employed that does not permit too large grains to emerge within the material (see, Fig. 2). The force field acts as if it would assure the uniform squeezing of the material from each space side, causing this way the small grains to occur at the expense of fine-graining and densification conditions expected to manifest in parallel [2, 7]. By applying so-described procedure, one can obtain materials with a superplastic behavior (such as the ones concerning Al-type nanomaterials [1, 2]) or materials with improved superconducting properties (such as YBaCuO ceramic materials created by top-seeded multilayers method [7]). This force field would modify accordingly the SD-drift function (Eq. (5)), in a way of

$$B_{\pi}(R, t \to \infty) = -\left(\frac{d}{dR}(\Phi(R) + E_{\pi})\right) \times \frac{D(R, t \to \infty)}{k_{\mathrm{B}}T}, \tag{7}$$

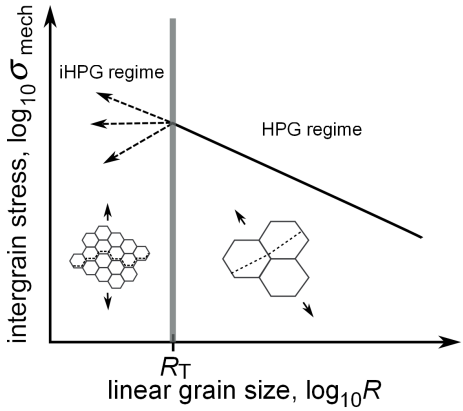

Fig. 1. Diagrammatic depiction of intergrain stress σ_{mech}, Eq. (6), as a function of linear grain size $R \geq R_0$. If grain size is greater than some threshold value R_{T}, it obeys the simple HPG scaling relation for $R \gg R_{\text{T}}$, but if it goes down beyond this point ($R \sim R_{\text{T}}$), then polycrystalline material enters a superplastic iHPG regime (dashed lines show only examples of possible scenarios). In iHPG regime, one expected to have $R_{\text{T}} \gtrsim R_0$ due to high-pressure damping of the growth mentioned [2].

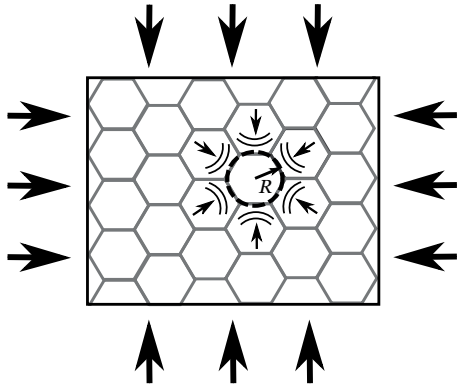

Fig. 2. High pressure, applied from every direction, does not permit too large grains to emerge within the material ($R \sim R_0$). (Note that hexagonal grains are only an ideal case and are drawn only as an "equilibrium" honey-comb type example.)

wherein in the case of $R \sim R_0$ and $\nu_{\text{HPG}} < 0$ [21], one takes the pressure-involved positive energy $E_\pi > 0$, as to achieve the corresponding high-pressure (or, hyper-pressure *viz* severe plastic deformation [20]) nearly macroscopic effect on the grain-size magnitude, and also, on the stresses' accumulation, according to Eq. (6). Otherwise, one had to accept non-positive E_π-level. By $E_\pi = 0$, one indicated natural (nano)colloid-type

matter aggregation with absence of an external force field [6], whereas with $E_\pi < 0$ (hypo-pressure or depressurization effect) one is going to land on fairly coarse-grained material [3, 12]. In external shock-pressure conditions nonequilibrium theory of vacancies, addressing the melting phenomenon in terms of (dis)continuous phase transition phenomenological rationale of Landau type, has recently been proposed [22, 23].

To sum up, in part, it is claimed that by means of manoeuvring with SD context, yielding some average value of the grain size ($R \equiv R(t)$) [8, 15], introduced then to the growing rule

$$\frac{dR(t)}{dt} \propto \left(\frac{1}{R(t)}\right)^{\mu_{\mathrm{NG}}}, \tag{8}$$

(basically, also with a stochastic account included [4, 16]), we are, in principle, able to get explicit solutions of them [12, 13], at some $t \simeq t_{\mathrm{s}}$ too, and when including the modified form of $B_\pi(R, t \to \infty)$, Eq. (7). Bear in mind that $\mu_{\mathrm{NG}} \geqslant 0$ stands for a characteristic growth exponent [13, 15]. For example, if $\mu_{\mathrm{NG}} = 0$, a growing, mass-convection-like pattern should emerge [8, 13]. If, in turn, $\mu_{\mathrm{NG}} > 0$ a plethora of characteristic growing outputs may arise, as, for example, the diffusional one with $\mu_{\mathrm{NG}} = 1$ [4, 12]. For $\mu_{\mathrm{NG}} > 1$, some subdiffusive slowly evolving patterns are legitimate to occur, *etc.* [12]. (The case of $\mu_{\mathrm{NG}} = 0$ at $t \to \infty$ in conjunction with HPG relation can be achieved too [10].) Then, we may resort to the HPG type of approximation, given by Eq. (6), in order to estimate, within the scaling hypothesis, the accumulated stress field, distributed over the grain boundaries. (Outside the approximation, one has to mention additional effects such as grain-boundary sliding, rotational and/or translational grain movement, also other anomalous strengthening mechanisms [21].) It helps, in turn, identifying the real involvement of the time scale, and the processes that assist certain distinguishable time instants, resorting the main growing and structure-maturation effects, into the ones characteristic of the overall nucleation-growth (NG) phase transition [15], as has been proposed in [8], and elaborated in some FD context [9] in the subsequent section. Realize, however, that the present paper is addressed more to show up the basic fingerprints of the method applicable to polycrystalline complex-material and mechanical context *per se*, than to pay too much attention to the detail of any peculiar (soft) matter aggregation of interest published elsewhere [5, 6].

2.2. Related restricted-growth example coming from econophysics

Let us offer another quite a real-life econophysical example, qualitatively related to our problem. It has been inspired by a price-variation dynamic stock model by Bak *et al.* [24]. The model contains a certain number of

investors and/or traders. They can, however, be divided into two groups: rational and irrational ones (see, Fig. 3). Rational and irrational investors have different interests. The first ones are applying the fundamental analysis of shares prices and hence are using stock as an investment that reflects a real company's value (being often a long term investment). The second ones are using individual strategies to search for a profit (often in a short run). They both have different strategies and often different interests that cause stress and tension. Let us denote specifically here the number of rational investors by R_{I}[1], whereas the corresponding number of their irrational counterparts would read I_{I}. Thus, the total number of investors is given by $N_{\mathrm{I}} = R_{\mathrm{I}} + I_{\mathrm{I}}$, and can be large, $N_{\mathrm{I}} \gg 1$. Let us collect the R_{I}-investors in one big bubble, assuming that still $I_{\mathrm{I}} \gg 1$ applies. By buying and selling stocs, R_{I}-investors bubble can expand according to the Kelvin–Laplace (KL) law, and due to the pressure difference, $\Delta\pi$ [15], executed toward the environment.

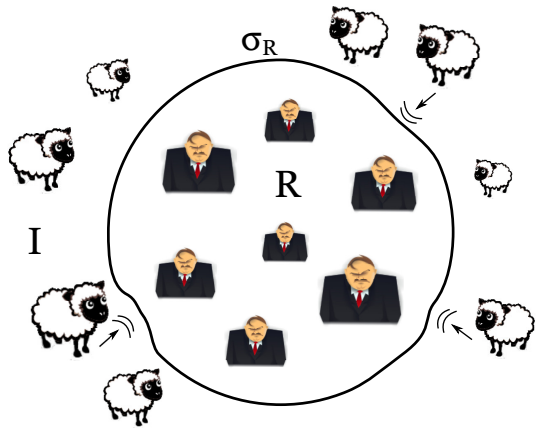

Fig. 3. Imaginative illustration of rational investors' bubble on which the irrational investors (sheep), due to their diffusion, put a pressure blocking this way the rational bubble's expansion. (See Sec. 2.2 for notation details.)

According to KL law [4, 12], the expansion of a spherical bubble of radius $R \equiv R(t)$ (in tree-dimensional Euclidean space) goes in time t as follows

$$\frac{dR(t)}{dt} = \frac{2\sigma_{\mathrm{R}}}{R(t)}\,, \tag{9}$$

where σ_{R} is the bubble's surface tension.

The I_{I}-investors perform their businesses somewhat "chaotically". They are allowed to diffuse over the spherical-bubble surface, blocking somehow

[1] Not to mismatch R_{I} with the grain radius, R, though both quantities can be seen analogous.

this way the rational bubble's expansion. Thus, their diffusion influences the value of σ_{R}, making it "diffuse". It can be shown that σ_{R} has to be very naturally a function of $1/R^2$ here. It is because one can present it as

$$\sigma_R = \frac{E_R}{4\pi R^2}\,, \tag{10}$$

with E_R being the mean-value energy accumulated within the R_{I}–I_{I} interface [15].

How does the diffusion influence plausibly the value of σ_{R}? It can do so by assuming that each of small I_{I}-bubbles may perform a diffusion driven growth [25], partly against the pressure-influenced growth of the bubble. Since the matter flux $J(R)$ involved in such growth along each of the radial R-directions is, according to Fick's law, inversely proportional to R, like $J(R) \propto 1/R$, thus the overall diffusion (causing "mater income") rate, has to be quantified by $-dJ(R)/dR \propto 1/R^2$, which corresponds to what has been given by Eq. (10), wherein E_R is going to be closely related to the diffusion constant D_{I}, namely $E_R \propto D_{\mathrm{I}}$, both of them depending on the stock "temperature", T_{IR} (hot- or cold-interface effect).

Combining then the mutual dynamic (opposite) action of R_{I} and I_{I} traders by inserting Eq. (10) to Eq. (9), one gets

$$\frac{dR(t)}{dt} \propto \frac{1}{R^3(t)}\,, \tag{11}$$

which yields a subdiffusive expansion tempo for R_{I}-bubble such as

$$R(t) \propto t^{1/4} \tag{12}$$

thus, resembling very much the capillarity-influenced evolutions of grains in polycrystals (the $(d = 3)$-case therein), *cf.* [12], *i.e.* if $\mu_{\mathrm{NG}} > 1$ is applied. The result (12) can be compared with a formula obtained by Bak *et al.* [24] for stock prices' variations Δp. They behave asymptotically at very long time scales as the ones scaling with a Hurst exponent of $H = 1/4$. Such $H = 1/4$-scaling has already been confirmed by means of 2D Monte Carlo computer simulation [26, 27]. In [28], the Hurst exponent was calculated for the shares prices using the local so-called Detrended Functional Analysis. It was compared with threshold values $1/4 \leq H_{\mathrm{threshold}} \leq 2/5$ in order to predict changes in trends. Several examples of $H < H_{\mathrm{threshold}} = 1/4$ were noticed. Let us believe that such econophysical analogy sheds also more light on what can dynamically arise at the I_{I}–R_{I} interface which is reminiscent of the grain (*viz* bubble) boundary. From our example it follows that stress (quantified in terms of diffusive surface-tension effect, see above) can spread along this territory, and the quantity $E_R \propto D_{\mathrm{I}}$ can presumably be thought of in terms of the energies for dislocations' motions addressed by Griffith [22, 23].

3. Fractional grain-growth and time-sensitive dynamics, and their correspondence with mechanically addressed Smoluchowski counterpart

Thus, according to the above mechanical-growing and related context invoked, in this section, we analyze for explanatory and comparative reasons the solution of the before announced, time-sensitive and superconducting-material NG equation which comes out from the Mullins–Von Neumann cellular-network (Voronoi) evolution [12] (see, [8] and Eqs. (5) and (9) therein)

$$ {}_0D_t^{\alpha} R_n = \delta_T \cdot c \left(\frac{n}{6} - 1 \right) , \tag{13} $$

where the operator ${}_0D_t^{\alpha}(\cdot)$ is a left Riemann–Liouville derivative [9], for $0 < \alpha < 1$ defined by

$$ {}_0D_t^{\alpha} f(t) = \frac{1}{\Gamma(1-\alpha)} \frac{d}{dt} \int_0^t \frac{f(\tau)}{(t-\tau)^{\alpha}} d\tau \, . \tag{14} $$

In Eq. (13), δ_T is a temperature (T)-dependent parameter which describes grain boundary thermodynamics, and is proportional to curvature of the grain (inversely proportional to grain size), c is a kinetic constant, and n provides the number of sides of the fairly polygonized polycrystal grain [8]. R_n denotes the radius of a superconducting domain. Realize that Eq. (13) is analogous to Eq. (8), and to some extent to Eq. (11), the former arising from SD context, especially for $\mu_{\mathrm{NG}} \neq 0$. The emergence of Riemann–Liouville derivative in Eq. (13) results in the fact that upon evolution the grain growth at time t is also affected by how it has evolved since time $t = 0$. Thus, we have implemented here the memory effect [30]. We are interested in solving this equation. We can use the composition rule of the fractional integral of the order α with fractional Riemann–Liouville derivative of the order of α. Alternatively, we can use Laplace transform technique to Eq. (13). The solution takes a form of

$$ R_n(t) = \delta_T \cdot c \left(\frac{n}{6} - 1 \right) \frac{1}{\Gamma(\alpha+1)} t^{\alpha} + \frac{C}{\Gamma(\alpha)} t^{\alpha-1} , \tag{15} $$

where $C = \left[{}_0I_t^{1-\alpha} R_n(t) \right]_{t=0^+}$ (taken in the following as small value) and symbol ${}_0I_t^{1-\alpha}(\cdot)$ is the fractional integral of the order of $1 - \alpha$. The second term from the right-hand side of Eq. (15) represents non-local initial

condition[2]. We find, as other authors, that there is no known physical interpretation for such types of initial conditions [9]. Now, let us focus on the late-time limit which means that $R_n(t \simeq 0) \sim 0$ (at some finite α). It then enables to postpone the second term in right-hand side of Eq. (15). The problem with physical interpretation can be solved, if we make an assumption about our function $R_n(t)$, that belongs to the class of one differentiable functions in the ordinary sense. Then, we can use the relation [9] between derivative defined by Eq. (14) and the Caputo derivative [31] defined for $0 < \alpha < 1$ by the formula

$$ {}_0^C D_t^\alpha f(t) = \frac{1}{\Gamma(1-\alpha)} \int_0^t \frac{1}{(t-\tau)^\alpha} \frac{df(\tau)}{d\tau} d\tau \,. \tag{16} $$

Then Eq. (13), with assumption $R_n(t \simeq 0) \sim 0$, can be written in the following form of

$$ {}_0^C D_t^\alpha R_n(t) = \delta_T \cdot c \left(\frac{n}{6} - 1 \right) . \tag{17} $$

When using the Laplace transform method, the solution of Eq. (17) can be obtained as

$$ R_n(t) = \delta_T \cdot c \left(\frac{n}{6} - 1 \right) \frac{1}{\Gamma(1+\alpha)} t^\alpha \,. \tag{18} $$

Function $R_n(t)$ parametrically depends on the temperature [8] and this is a crucial physical parameter which one can control in some practical or technological applications [32].

Transforming Eq. (13) by acting on its both sides with the Riemann–Liouville derivative of the order of $1 - \alpha$ and using the composition rule for this derivative, and postponing the second term in right-hand side of Eq. (15), we obtain the following relation

$$ \frac{d}{dt} R_n(t) =_0 D_t^{1-\alpha} \left[\delta_T \cdot c \left(\frac{n}{6} - 1 \right) \right] . \tag{19} $$

Equations (13)–(19) treat R_n as a deterministic quantity, which is going to change its size according to Eq. (13) or Eq. (17). However, an indication

[2] Bear in mind that the Eq. (15) expresses, in general, a capability of two different behaviors in two corresponding time domains. At some fixed α, specifically taken at $\alpha = 1/2$ (specifically, within diffusive mode, *cf.* Eq. (18)), the first term from right-hand side of Eq. (15) is preserved at some long-time limit, while the second prevails at an early stage of the material formation. It gives a tight analogy to what we got from applying a HPG criterion, *cf.* Eqs. (6) and (8). Further, taking the limit of $\alpha \to 0$, the second term of Eq. (15) but exclusively at early times is emphasized. The late-time limit of $\alpha \to 0$ yields a termination of the growing process because according to Eq. (15) $R_n \to$ const. Analyzing the limit of $\alpha \to 1$, a constant-rate material formation is favored, realized as revealed by [8].

of a statistical model that explains Eq. (19) is at our disposal and conforms to our overall growth *vs* mechanical late-time response scenario [4].

The form of Eq. (19) give us hint how to obtain theoretical explanation of Eq. (13). Returning to the introductory remarks of Sec. 2 of this work, we wish to recall that we are considering the phase space $(0, R)$ of main characteristic linear grain/domain size.

There exists also the probability density $P(R, t)$, which is described on the $(0, R)$-axis. In the discrete case of the phase-space considered, the vector of grain sizes $\hat{R}$, and the vector of its probabilities $\hat{P}(t)$, arise. Taking into account the form of the Eq. (19), we recall suitably the generalized master equation [33]

$$\frac{d}{dt}\hat{P}(t) =_0 D_t^{1-\alpha}\left[\hat{V}\hat{P}(t)\right], \tag{20}$$

wherein $\hat{V}$ is a matrix of constant numbers $\hat{V}_{ij}$.

In this discrete issue, we can evaluate the average

$$\left\langle \hat{R}(t)\right\rangle = \sum_{i=1}^{N} \hat{R}_i \hat{P}_i(t)\,, \tag{21}$$

and calculate how it is changing in time

$$\frac{d}{dt}\left\langle \hat{R}(t)\right\rangle =_0 D_t^{1-\alpha}\left[\sum_{i=1}^{N}\sum_{j=1}^{N} \hat{R}_i \hat{V}_{ij} \hat{P}_j(t)\right] =_0 D_t^{1-\alpha} \Lambda(t)\,. \tag{22}$$

The function $\Lambda(t)$ depends on time except of situations in which it equals zero (equilibrium state). In a model with evolution, Eq. (20), there is an assumption staying behind it, that the changes of $\hat{P}(t)$ are performed by the transition matrix $\hat{M}$ of constant numbers. If the matrix $\hat{M}$ acts once during time interval $[t_1, t_2]$ on a vector $\hat{P}(t_1)$, then we get new vector $\hat{P}(t_2) = \hat{M}\hat{P}(t_1)$. The period of time when matrix $\hat{M}$ does not act on probability vector $\hat{P}(t)$ is taken from some distribution $\psi(t)$. If the waiting time gets on a form of $\psi(t) = 1/\tau \exp(-t/\tau)$, then between matrices $\hat{M}$ and $\hat{V}$ there exists a simple relation $\hat{V} = (\hat{M} - \hat{1})/\tau$ [34], where $\hat{1}$ is an identity matrix and $\tau > 0$. This is equivalent to the master equation in a well-known form, namely

$$\frac{d}{dt}\hat{P}(t) = \hat{V}\hat{P}(t)\,. \tag{23}$$

However, if we assume the generalized master equation in a form of Eq. (20), then we keep the relation between the involved matrices $\hat{M}$ and $\hat{V}$ (here one has to indicate $\tau = 1$), but with a new waiting time whose Laplace transform

gets a form of $\tilde{\psi}(s) = 1/(1+s^{\alpha})$ (see some details in [33] for two-dimensional case). Taking into account properties of master operator $\hat{V}$, we can write

$$\hat{V}_{ii} = -\sum_{j \neq i} \hat{V}_{ji}\,. \tag{24}$$

Then, it is not complicated to write down Eq. (20) in a form of

$$\frac{d}{dt}\hat{P}_i(t) =_0 D_t^{1-\alpha}\left[\sum_{j\neq i}^{N}\left(\hat{V}_{ij}\hat{P}_j(t) - \hat{V}_{ji}\hat{P}_i(t)\right)\right]. \tag{25}$$

In order to move to a continuous variable R, we do perform a standard substitution within Eq. (25). Vector $\hat{P}(t)$ is replaced by the function of probability density function $P(R,t)$ which described the density of grain size R at time t. The terms $\hat{V}_{i,j}$ are replaced by a function $W(R|R')$ and summation is adequately replaced by integration

$$\frac{\partial P(R,t)}{\partial t} =_0 D_t^{1-\alpha}\left[\int_0^{+\infty} W\left(R|R'\right)P\left(R',t\right) - W\left(R'|R\right)P(R,t)dR'\right], \tag{26}$$

i.e., having, in fact, incorporated at the r.h.s. detailed-imbalance conditions. The next transformations of Eq. (26) are rather standard. For $\alpha = 1$, one can find it in [35]. The function $W(R|R')$ is replaced by $\tilde{W}(R', \Delta R)$, a function expressing a change of grain size $R - R' = \Delta R$ when commencing with a grain size R'. For the rest of functions, we write $W(R'|R) = \tilde{W}(R; -\Delta R)$ and $P(R',t) = P(R-\Delta R, t)$. Also we change the variable of integration R' to ΔR and the limits of integration to $(-\infty; +\infty)$. There are other assumptions about the functions. One of them is that $\tilde{W}(R'; \Delta R)$ as a function of ΔR changes very fast, but it changes very slowly as a function of R'. We need to use approximation $P(R-\Delta R; t) \sim P(R; t)$ and the Taylor series for $P(R - \Delta R; t)\tilde{W}(R - \Delta R; \Delta R)$. We also assume that $\tilde{W}(R; \Delta R) = \tilde{W}(R; -\Delta R)$. All those assumptions applied to the Eq. (26), and complemented by some standard formulae

$$A(R) = \int_{-\infty}^{+\infty} \Delta R W(R; \Delta R) d(\Delta R) \tag{27}$$

and

$$B(R) = \int_{-\infty}^{+\infty} \frac{\Delta^2 R}{2} W(R; \Delta R) d(\Delta R) \tag{28}$$

are causing to provide the following

$$\frac{\partial P(R,t)}{\partial t} =_0 D_t^{1-\alpha}\left[-\frac{\partial}{\partial R}A(R)P(R,t)+\frac{\partial^2}{\partial R^2}B(R)P(R,t)\right]. \tag{29}$$

This equation is known as a fractional diffusion-advection equation [36, 37], wherein $A(R)$ has customarily got an interpretation of expressing proportional to a field of velocity which would depend on the size of a grain (or, domain upon growth). According to continuous time random walk (CTRW) theory, in such interpretation Eq. (29) describes such microscopic situation, that the grains do grow in a discrete way (or, phase space). Between two successive changes of grain sizes, a potentially keen-to-growth grain is waiting. In this model, there is also inhomogeneous velocity field $V(R)$ and a certain characteristic advection time τ_{a}. When grain would change its size, it is adjusted by the presence of the drift velocity through the time of advection. If in standard CTRW we address to mark by $\psi(\Delta R, \Delta t)$ a density of change of grain size ΔR and a waiting time Δt between the corresponding changes, then in terms of velocity in our model, one could write $\psi(\Delta R - \tau_{\mathrm{a}}V(R), \Delta t)$.

In the simplest case when velocity field is homogeneous $A(R) = \text{const.}$ and $B(R) = \text{const.}$, we can obtain the following relation

$$\frac{\partial}{\partial t}\langle R(t)\rangle =_0 D_t^{1-\alpha}A\,, \tag{30}$$

wherein

$$\langle R(t)\rangle = \int_0^\infty RP(R,t)dR\,. \tag{31}$$

Analogous relation for the first moment of the $P(R,t)$-involved process can be found in [11, 12] but exclusively for interpretation of $A(R)$ as a constant force in the subdiffusion process. If we wish to identify $\langle R(t)\rangle$ with $R_n(t)$ in Eq. (13), then Eq. (30) is equivalent to Eq. (19). So, we can see that

$$A = \delta_T \cdot c\left(\frac{n}{6}-1\right), \tag{32}$$

cf. Ref. [8]. One can state, that result (13) is perceivable on the ground of so-introduced fractional diffusion-advection process in the continuous phase space.

Due to the obvious property of the Riemann–Liouville derivative that ${}_0D_t^{1-\alpha}0 = 0$, one can find stationary solution of Eq. (29) by assuming $B(R)$ as a constant [11]. It has a form of

$$P_{\mathrm{st}}(R) = \exp\left(\frac{1}{B}\int_{R_0}^{R} A(r)dr\right), \tag{33}$$

which, in general, coincides well with the Boltzmann-type stationary state's formal one-energetic-barrier depiction [6], see above.

4. Summary

Let us summarize the present study in the following way. Namely that:

- the main effort of the underlying work has been to link the suitably addressed late-stage growing (super)material's conditions [1] with their expected though still putative mechanical-stress involving counterparts [3], in order to support modeling of materials with desired properties such as superplasticity or superconductivity (see, Sec. 2.1);

- the HPG type simple *vs* inverse mechanical relations, expected to occur [4], came out from the late-stage and mature enough evolutions of either superplastic [2, 20] or superconducting [7, 32] model materials (*cf.*, Eq. (6));

- some qualitatively depicted mechanical-stress-like tensions [20] at the suitable border of opposing domains' growth can be recast comparatively by means of an econophysics-addressing trader *viz* investor's market example [24], *cf.* Eq. (9), with a big *vs* small (stock [28]) bubble concurrence [26] involved (those tensions may cause via $H = 1/4$ a change in shares prices trend [28]);

- the mechanical-stress action upon mature growing condition can be reconsidered when the subtleties of the FD-involving time scale can be applicable at length [38], as has been realized in terms of superconducting material's (whole time scale) emergence [8], *cf.* Eq. (13);

- the overall SD-type (thermo)dynamic picture [8] staying behind, pretends to unify purposely the very physical fact that late-stage object's (physico- or econo-physical domain) growing conditions do introduce ultimately some interesting mechanical-field assisted HPG-type peculiarities coming from the nature of the defects-containing overall process [18, 22], and supported by the FD-framework [11].

In the last word, let us indicate that within the framework of the statistical-mechanical, and sometimes mean-field type overall picture addressed [8], a qualitative quasi-unification of the material- and other, such as econophysical properties [28] of the underlying grains-containing system, have all together been utilized in order to create a comprehensive view of the mesoscopic mechanically-engaged, and memory-involved [28, 33], also viscoelastic [30], complex-system aggregations of interest [5, 6, 25]. As a

future work, coming out from our study, one might offer finding out the precise correlation scheme between μ_{NG} and α exponents, as has already been suggested by [4, 8].

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