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Simple example of structure versus property relationship applied to a reduced-friction biosystem, a quite personal opinion

Adam Gadomski

Department of Modeling of Physicochemical Processes, Institute of Mathematics and Physics,
University of Technology and Life Sciences, Kaliskiego 7/421, 85796 Bydgoszcz, Poland

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ABSTRACT

Structure versus property (small-scale) relationship enters when something interesting is going to happen in a biosystem. This special-type “happening” is actually appearing to be manifested at both micro- and mesoscopic levels of always productive soft-matter organization under dynamic response, especially the one characteristic of the articular cartilage—an efficient, designed-by-nature multi-membrane, and virtually, with-ion-channels equipped, absorber and load relaxor.

1. Introduction

Imagine a biologically legitimate absorber under load consisting of two “attacking” upper and lower (porous and rough) solid surfaces and a complex layered fluid in-between, (cf. Scherge and Gorb, 2001). A fundamental question appears: which is the structure of the layers in-between, assumed that the solid surfaces are dealt with as self-consistent, “noninvading” solid surfaces, the role of which is meant exclusively in transmitting either normal or lateral (shear) effect on the complex layered structure in-between? For the purpose of the underlying study, let us assume that the complex fluid in-between is a ‘planar layered’ tissue, in which the surface active phospholipids (SAPLs), being at equilibrium in its elongated state with its synovial-fluid remaining counterpart, do exist, initially as bilayers, or multilayers (Israelashvili, 1991), cf. Fig. 1. Amongst phospholipid surfactant molecules, there appear water molecules: they can be dipoles (out of equilibrium) or dissociated H^+ and OH^- ions (appreciably close to equilibrium). Other components of the complex fluid layered in-between structure are equally important molecules such as hyaluronic acid, glycoproteins, proteoglycans, aggregacens, collagen fibers, etc., to mention but a few (Scherge and Gorb, 2001). They are, of course, quite specific, thus relevant, since they make the system as being virtually able to bear the applied external load. What remains to be crucial, however, appears to be an attractive and experimentally justifiable supposition (Gadomski et al., 2008) that the system reorganizes under load (or, shear, or both) into SAPL nanochannels involving mesostructures, in particular micelles, expected to occur in the synovial interlayer already mentioned. In what follows, let us convince the reader that an open–closed SAPL channel dynamics, with the lightest H^+ ion-channel passages, being engaged, appears to be the case worth reconsideration, especially in view of the theories on articular-cartilage functioning offered so far (Scherge and Gorb, 2001).

2. The dynamic model at mesoscale

As introduced in a recent letter (Gadomski et al., 2008), the model includes a well-combined and naturally arising dynamics of emergence of micellar (quantified by a dependent variable, $\varphi - a$ concentration of SAPLs in its organized viz micellar state) microstructures at the expense of their non-micellar (layered) counterparts, designated by ρ, see below. The fundamental coupling between φ and ρ is assumed to be linear (Gadomski, 1997), being reminiscent of a dynamical-system coupling (Shpenkov, 1995), attributed typically to a linear oscillator, namely:

$$y = ax + b, \tag{1}$$

wherein $y = \dot{\varphi}$ (if $x = \rho$) or $y = \dot{\rho}$ (if $x = \varphi$), the over-dot denotes ordinary differentiation over time t and a, b are some properly adjustable parameters (Gadomski, 1997), addressing the role of external SAPL sources (note that the system we consider is an open thermodynamic system, also due to the porosity of the solid

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E-mail address: agad@utp.edu.pl.

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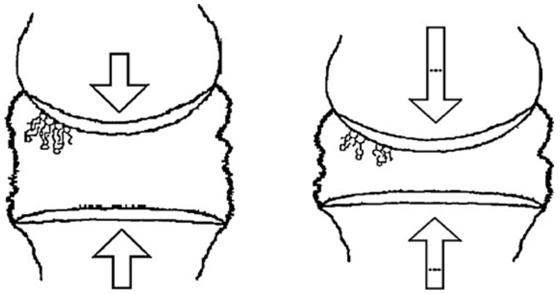

Fig. 1. Schematics of a model articular cartilage (i) under weak load, left; (ii) under strong load, right. Upper and lower solid surfaces, dealt with the normal load (arrows) are depicted, leading to getting the interlayer squeezed – the interlayer is represented for simplicity reasons by the surface active phospholipids (SAPLs) matter, typically consisting of amphiphilic lipid molecules such as *DPPC*. They, having stuck to the upper solid layer (far oversimplified), are depicted in such a way as to mimic close (left) versus open (right) channel-formation dynamics in the interlayer, seen as a "white matter" in which many small-scale effects (Mate, 2007) may emerge. To fasten the cartilage, collagen fibers are designed by nature – they are drawn as curvilinear threads linking the solid, typically rough and porous, surfaces (Scherge and Gorb, 2001).

surfaces, constituting it), by-SAPL-caused defect formation, thus, either creation or annihilation effects, present in the interlayer, assisted by water ions (and, dipoles), etc. (Gadomski et al., 2008). This linear coupling is, however, not a thing that readily matters—it mainly helps to understand the system's (typically quasi-periodic) behavior in relatively simple terms. What matters substantially originates from the complex time, or load's duration, dynamics, and appears explicitly in a form of an Avrami–Kolmogorov phase-change resembling formula (Gadomski, 1997), namely:

$$\dot{\varphi} = \varphi_s + \text{const.} \times K(1-\varphi), \tag{2}$$

wherein the close-to-solid-surface source $\varphi_s \propto \rho$ in late-time-dynamics approximation (as above, the over-dot means differentiation over time). The dynamics of the ρ-field (a concentration of SAPL in its non-micellar state, close to both upper and lower surfaces of the cartilage, cf. Fig. 1) is governed by defects-competition dynamic equation to be found elsewhere (Gadomski, 1997; Shpenkov, 1995). But we do not wish to discuss it within the scope of the paper. What is truly worth stressing appears to be that the friction-dynamics coefficient K undergoes its very peculiar, toward reduced-friction designated (thus, legitimate) dynamics, namely (Gadomski et al., 2008; Gadomski, 1997):

$$\dot{K} = -\text{const.} \times K(\kappa^{-1} - \kappa), \tag{3}$$

wherein κ is a K-dependent algebraic function, see Ref. Gadomski et al. (2008). All peculiarities of the underlying model (Gadomski, 1997), applied at a mesoscopic (intermediate) level of matter organization, have been revealed in a separate study on tribo-polymerization (Shpenkov, 1995). Notice, however, that when looking more closely at Eq. (3) one sees that a stationary state for the friction to prevail, thus $\dot{K} = 0$, appears when either $K = 0$ (high-friction case of no interest in this study, considered elsewhere (Gadomski, 1997; Shpenkov, 1995)), or $\kappa^2 = 1$, i.e. the low-friction case of special interest in this opinion type short paper; note that the dynamic friction coefficient is thought to be an inverse of K (Gadomski et al., 2008). What is the plausible extension of such a mesoscale description can be seen in what follows, thus, when some microscale arguments are legitimate to enter, and the small-scale tribology can be introduced (Mate, 2007).

3. The extension toward microscopic view

The extension of the model into microscale has already been proclaimed. But, nevertheless, a physical reality must properly keep the pace. As revealed by a hypothetical study (Gadomski et al., 2008), the clue of the underlying dynamics lies in choosing properly the dynamical kernel K of the virtual high-to-low friction-involving transformation, more toward $\kappa^2 = 1$, thus, toward reduction of friction, than toward $K = 0$ state of high-friction regime (Shpenkov, 1995). We opt for a plausible scenario (Gadomski et al., 2008) that at $\kappa^2 = 1$ structural reorganization of the interlayer occurs. From the microscopic point of view this implies to have, on average, the SAPL molecules squeezed under the applied load (the so-called open-channel state). This small-scale-based observation makes a room for: (i) emergence of interspaces between the micellar mesostructures as possible to form in a channel-like manner; (ii) appearance of ion streams: the passage of H^+ ions, viz protons, as the lightest, thus heaving the biggest kinetic energy, contributing to the total interlayer's momentum, then, via the second Newton's law, subjected to the solid surface of the cartilage, to the (interstitial) pressure acting on it, while changing even slightly the load's duration, looks a legitimate case for further experimental reconsideration (Hills, 2000a,b; Israelashvili, 1991; Scherge and Gorb, 2001). For details of this microscopic, viscosity-change involving mechanism, also assisted effectively by otherwise negatively pronouncing electrostatics of the solid surface(s) of the cartilage one is encouraged to look into (Gadomski, 1997; Gadomski et al., 2008).

Thus, from the recently performed study, (cf. Gadomski et al., 2008) and Refs. therein, it follows that complex architecture of the layered multi-structure in-between really matters. As far as our quite hypothetically oriented address on this particular reduced-friction system is concerned it matters mainly from a practical point of view, namely that the least-dissipative model of purely Debyean character (thus, pointing indirectly to healthy knees and hips), is really the foremost case that emerges. Certain pathological, e.g. osteoarthritis involving quite frequent "exceptions" could then be examined while departing from this model (Hills, 2000a,b) even slightly, this way violating a theoretically proposed, and on random-walk-conception-based argument (Shpenkov, 1995), thus, a basic structure–property relationship inferred from microscale considerations under Debyean (exponentially fast—this type of relaxation will certainly drop down with the age or over-usage of the absorber/articular cartilage, an equally interesting point to embark) relaxation of the cartilage's material, namely (Gadomski et al., 2008):

$$3\gamma + \delta = 2, \tag{4}$$

wherein γ is the by-SAPL-constituted structural elasticity small-scale parameter, taking on proper values when the SAPL molecules get squeezed or not (i.e., when close-channel effects dominate), whereas δ stands for the ratio of a fractal dimension of the temporarily formed nanochannel, and the fractal dimension of the proton's typical trajcetory, the latter being generally envisaged by a self-avoiding random-walk concept as the most effective case. (Notice formally that these both parameters enter K, the – as well call it – tribomicellization, small-scale sensitive (Mate, 2007) kernel.) This channel is basically made up of SAPL matter, and the random-walk exponent represents either enhanced, or normal, or finally, slow diffusion of the protons along the channel (Gadomski et al., 2008), all of them contributing, depending on the load's magnitude, to the interstitial pressure in the interlayer. For the self-avoiding random-walk instance, depending on the (Euclidean) space dimension, d, one expects to have the random-walk dimension, d_{SARW}, to be $d_{\mathrm{SARW}} = (d+2)/3$ according to the famous Flory–Fisher mean-field fairly approximate estima-

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tion. Presumably, a notification upon existence of the self-avoiding random-walk measure could be viewed as some relaxation and facilitated biolubrication efficiency measure, clearly favoring the case of $d_{\mathrm{SARW}} = d = 1$ a topic demanding further exploration, correlated efficiently with adequate experimental-data acquisition. As a consequence of the above conveyed, the formula (4) is uncovered to be quite a simple example of the small-scale structure–property relationship, suffered virtually by a model articular cartilage (Fig. 1) under normal or lateral load in most effective (Debyean) material relaxation conditions. Otherwise, one would expect departures from this low-dissipation type of relaxation behavior, manifesting in standard viscoelastic system such as rubbers, and the likes. Such departures would be detectable effects at meso- and, of course, macroscale (governed by Coulomb–Amontons law), finally, showing up either some normal behavior or abnormalities, describable as mechanical-relaxation concerning and reduced shock-absorption revealing pathologies.

4. Conclusion

In the light of what has been presented above, one sees that what truly matters is foreseen, (cf. Ref. Gadomski et al., 2008), to be microstructure of the interlayer, manifesting between two solid surfaces of the cartilage under load or when load is removed, thus, when the by-small-scale mediated relaxation comes into play. Of special importance appears to be, however, the type of change of the microstructure, when the ion-channels dynamics is superimposed on it. We see quite natural that such meso- and microstructural mechanism of the confined matter organization under external “pressurizing” factor may shed quite new light on the existing substance of studies on this practical biomedical subject matter (Chen et al., 2007; Scherge and Gorb, 2001; Hills, 2000a,b; Mate, 2007; Israelashvili, 1991). There is no doubt that this overall issue seems to be open for an experimenter to cope with.

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References

Chen, Y., Crawford, R.W., Oloyede, A., 2007. Unsaturated phosphatidylcholines lining on the surface of cartilage and its possible physiological roles. J. Orthopaedic Surg. Res. 2, 1–6.

Gadomski, A., 1997. Description of the kinetics of a model tribopolymerization process. J. Math. Chem. 22, 161–183.

Gadomski, A., Pawlak, Z., Oloyede, A., 2008. Directed ion transport as virtual cause of some facilitated friction-lubrication mechanism prevailing in articular cartilage: a hypothesis. Tribol. Lett. 30, 83–90.

Hills, B.A., 2000a. Role of surfactant in peritoneal dialysis. Perit. Dial. Int. 20, 503–515.

Hills, B.A., 2000b. Boundary lubrication in-vivo. Proc. Inst. Mech. Eng. 214, 83–94.

Israelashvili, J.N., 1991. Intermolecular and Surface Forces. Academic Press/Elsevier, Amsterdam.

Mate, C.M., 2007. Tribology on the Small Scale. Oxford University Press, Oxford.

Scherge, M., Gorb, S., 2001. Biological Micro- and Nanotribology. Nature’s Solutions. Springer, Berlin, chap. 3.2.2, pp. 85–94.

Shpenkov, G.P., 1995. Friction Surface Phenomena. Elsevier, Amsterdam, pp. 165–172.

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