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Deformable cell and deformable tissue as an area for application of nanoscale mechanics

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Abstract

Materials undergoing deformation based on various mechanisms are frequently applied to manufacturing of artificial muscle actuators. In this paper we introduce a methodological step towards more precise determination of investigation object related to such actuators. One defines a deformable cell and a deformable tissue in order to indicate which functions of such objects should be integrated for further applications. One accentuates role of nanoscale models of mechanics of materials as important on way towards design of the deformable cells.

Keywords: Artificial muscles; Deformable cell, Nanoscale mechanics

1 Introduction

In last years we observe a tendency to transition of engineering to smaller and smaller scales in comparison with traditional large scale constructions like engines and so on. This is manifested by increasing role of physics, chemistry, material sciences and mathematics for engineering. In particular, ability to carry out complex numerical simulations leads to automatization of the design process. Above concise discussion generates the next question: where should we go with development of engineering. The natural answer suggests a tendency to more precise design. It means just creation of better physical foundations for equations of mechanics applied in engineering as well as transition to smaller scale with design of

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constructions. Nowadays, an outstanding manifestation of this tendency is promotion of nanotechnology.

An interesting area where decreasing of scale in design takes place is robotics. In particular problems related to motion of robotic systems and their control with finer precision with respect to forces and dynamics are important. Power source and power transmission during motion generation is of key importance. This is related especially to precise dynamics as well as forces induced by such a dynamics in environment.

In order to solve above problems one investigates for instance artificial muscles. They are constructed on many ways using shape memory alloys, contractile polymers, ionic-polymer metal composites and many other materials. The term "artificial muscle cell" is introduced in order to accentuate analogy with biological mechanisms of motion which is characterized just by fine controlling and sensitivity. One expects that by mimicking biological systems of motion we obtain robots which would have similar properties.

In order to introduce a methodology of investigations in the field of design of finer system of motion which would be able to imitate biological motion we should define some elementary concepts. The term "artificial muscle cell" is such an elementary concept. This term is well understood with respect to intention.

Usually one considers a deformable element composed of a material which has a controlling parameter. Relations between forces and deformation are predominantly investigated for such systems. However, whole problem of application of deformable element and its integration with a structure ensuring its functionality is not so carefully investigated. Consequently, in order to carry out theoretical descriptions of controlled deformable systems as well as well directed to this end experiments, we should define a unit corresponding to artificial muscles more precisely for further investigations. We should elucidate what we expect from such a type of cell.

The term "artificial muscle cell" is closely related to biology. In practice, in application of controlled deformable elements, we are not sure whether applications will always similar to muscles. Therefore, this name should be more abstract and directly associated with the function of the cell. The term "deformable cell" is more general and also more abstract. Class of such cells can be perhaps too large. We could consider for instance a piston engine as a deformable cell. However this is not rather our intention. Therefore, the deformable cell, which is in a perspective seen as rather small object, should be responsible for a simple motion as possible. Such a motion is easier for controlling. Then, more complex motions would be associated with a system of deformable cells which we call the deformable tissue.

In this paper we introduce a methodological step which consists in defining

deformable cell as well as a tissue of deformable cells in order to enable systematization of both theoretical and experimental investigations in this area. In particular one accentuates importance of nanoscale mechanics for description and design of such systems.

2 Characterization of deformable element of the cell

Deformable elements can be produced by various methods and materials. In this section we try to express properties of the a deformable cell which are the most characteristic. We assume in general that the deformable cell contains several subsystems which will be discussed in what follows. However, the main subsystem is associated with deformation.

Let us assume that motion of the deformable subsystem is characterized by a set of generalized coordinates $q = \{\mathbf{q}_i\}$ and forces $f = \{\mathbf{f}_i\}$. We can introduce a reference configuration determined by Q and displacements defined as $u = q - Q$ representing a finite set of degree of freedom. We introduce the term body for our deformable subsystem.

Let us consider the manifold \mathcal{M}_u which is a set of all admissible displacements of our body. Let us introduce also a submanifold $\mathcal{M}_R \subset \mathcal{M}_u$ of all displacements describing rigid motion of the whole body.

We introduce an equivalence relation \approx_R in \mathcal{M}_u . Then, two displacements u, u' are equivalent if they differ only by a rigid motion of the whole body. The manifold \mathcal{M}_u can be expressed as a fiber manifold considered as a generalized Cartesian product in the following form

$$\mathcal{M}_u = \mathcal{M}_D \times_f \mathcal{M}_R, \quad (1)$$

where \times_f stands for a symbol of generalized Cartesian product operation, \mathcal{M}_D is a fiber chosen for instance for 0 element of \mathcal{M}_R . Elements of the manifold \mathcal{M}_D are called deformation of our body. Such a manifold can be identified also with the quotient space given by

$$\mathcal{M}_D = \mathcal{M}_u / \approx_R. \quad (2)$$

Extensive discussion of deformation can be found in [1] for instance.

We express motion of our body by the equation

$$\Psi_i(\{\mathbf{u}_{fj}\}, U) + \mathcal{I}\ddot{\mathbf{u}}_i = \mathbf{f}_i, \quad (3)$$

where $u_f = \{\mathbf{u}_{fj}\} \in \mathcal{M}_D$, $\ddot{\mathbf{u}}_i$ is the second order time derivative of \mathbf{u}_i , Ψ_i represents internal force in the body corresponding to i -th degree of freedom and \mathcal{I} represents inertia characteristics in a generalized sense.

The function Ψ_i represents constitutive equations for material of deformable element. Such constitutive equations can have a variable which is interpreted as a control parameter. Let us mention temperature as a possible control parameter for shape memory alloys for instance. In general, we can admit that Ψ_i depends also on a set of internal state variables.

We have admitted that the force Ψ_i depends on a controlling parameter U . Consequently, the Eq. (3) should be supplemented by an equation describing evolution of controlling parameter

$$\dot{U} = \mathcal{A}_U(U, \chi, \eta), \quad (4)$$

where χ represents an impulse for activation of a controlling system which generates U and \dot{U} is a time derivative of U . Then, the system of variables η describes evolution of the controlling system. Such variables are introduced formally here in order to accentuate the fact that controlling system is a subsystem with its own properties.

We assume that the controlling parameter changes in a monotonic way $U \in [U_a, U_b]$ within an interval. Let $\mathcal{P}(\mathbf{u}_f)$ be a dominant property of our deformation. We postulate that $\mathcal{P}(\mathbf{u}_f)(U)$ also changes in a monotonic way which expresses our intention that the deformable cell realizes a simple motion. The property \mathcal{P} can express the elongation of deformable element for instance.

Summarizing, above description of motion of deformable cell is assumed as a simplified to the possible degree in order to express function of this element only. However, description of the whole physical phenomena in this element can be very complicated.

3 Subsystems of the deformable cell

Deformable cell contains a deformable element denoted here by S_D which induces deformation as the main function of the cell. However, our intention consists in construction of such an elementary object which would be deformable and additionally could be well controllable. We expect also that such elements can be incorporated into a larger system called the deformable tissue which would perform more advanced deformation and dynamics. Furthermore, the deformable cell should be a unit having an integrity which is protected against destruction.

The condition that elements can be joined follows that a part of the cell should be able to create joints. Consequently, we distinguish subsystem S_J which is responsible for joining the deformable cell with other cells and also with other objects which could cooperate with cells.

It is imaginable that the cell has its own power source or a system which fulfill this task. Therefore we distinguish the subsystem S_U which is responsible for

powering control functions. We have introduced a general equation for evolution of controlling parameter by (4).

Powering of the control needs a signal. The subsystem S_χ is responsible for activity of the system S_U .

The deformable cell can be destroyed by conditions which occur in an environment. Therefore, we have to ensure functionality of the cell. To this end we introduce the subsystem S_{ENV} .

In order to realize a feedback in controlling, especially more fine functions, it would be useful to endow the cell with a sensory subsystem controlling for instance a kind of stress or other parameters at small scale of single cell in comparison with whole tissue. Therefore, we introduce the subsystem S_{SENS} which should fulfill such a function.

Summarizing, our deformable cell can be expressed as union of subsystems

$$S_{DC} = S_D \cup S_J \cup S_U \cup S_\chi \cup S_{ENV} \cup S_{SENS} . \quad (5)$$

Deformable cells considered as so integrated systems as discussed above are rather not discussed in literature where main attention is devoted predominantly to the system S_D without integration of it with other functions. We encounter in literature many approaches to manufacturing of artificial muscle actuators.

The longest history has a pneumatic artificial muscle actuator [2]. The essential problem with pneumatic actuators is the requirement for bulky power sources apart from the actuator itself. This perhaps can be an obstacle for miniaturization within such a concept and creation of a tissue of such a kind of cells.

Another example which we encounter in literature is related to shape memory alloy actuators [3–5]. They have a great power density but the response time and the heat generation could be a problem in practical applications. This point of view represented in literature [23] suggests that shape memory alloys deformable subsystems S_D perhaps need just a miniaturization in order to improve dynamics associated with the heat controlling system. Then, the controlling subsystem S_U which should control a heat efflux towards S_D should be well defined within the deformable cell.

Let us note that magnetic shape memory alloys can be attractive with respect to method of controlling of deformation [6,7]. Perhaps, in such a case the system S_U could be easily integrated with S_D .

There are many materials which are applied as deformable elements and are based on larger molecules. Let us mention polypyrrolle mechanical actuators. Polypyrrolle is a conducting polymer which can undergo a volume change during electric stimuli. The deformation can also be induced by pH change, dopant ions or redox agents [8,9].

Electrostrictive actuators are also applied as actuators [10]. Let us note that

high voltage photoinductive switches considered in [11] can be considered as an example of integration of S_U with S_D .

Polymer gels are soft materials made of cross-linked three-dimensional polymer network containing solvent. Their ability to swell and deswell can be applied to making actuators [12]. Ionic polymer gels are also applied to this end [13]. In particular hydrogels are very important materials for discussed here applications [17–20].

Ionic polymer-metal composites (IPMC) are applied to various actuators including linear artificial muscle actuator using electric stimuli [14–16]. In particular we can observe appearing of tendency to produce something like S_{ENV} which consists in encapsulation [15] of part of working material on order to protect it against environment.

Deformable elements as actuators are also made of liquid crystal elastomers [21], and polymer nanocomposite materials (PNC) [22] considered within the category of electrostrictive materials.

We encounter in literature also a concept of application of electro-conjugate fluid for constructing deformable elements. Within this approach one discusses a concept of artificial muscle cell which is the most close to our concept of deformable cell. In papers [23, 24] one discusses also joints between cells and larger systems of such cells. The system S_U is represented by pair of electrodes which induce efflux of electro-conjugate fluid which in turn induces a deformation of the cell.

Within the papers [23, 24] we do not encounter any attempts to defining of the deformable cell on a general level. Above discussed papers show that introduced here concept of deformable cells can be useful.

Summarizing, we encounter in literature investigations which give evidence that subsystems distinguished within deformable cells are important. In particular we observe in literature some approaches which are associated with integration of subsystems with various functions. However, further development of such elements depends on taking into account of all aspects necessary for their application including cooperation of all subsystems.

4 Tissue of deformable cells

Let us consider a system of deformable cells $\{S_{DC\lambda}\}$, $\lambda \in \Lambda_{DC}$. Deformable cells indexed by means of λ need not to be identical. We assume that they are joined by means of subsystems $S_{J\lambda}$ which are corresponding parts of $S_{DC\lambda}$. We assume that subsystems $S_{J\lambda}$ are responsible for transfer of forces between deformable cells.

Let us assume that a part of $S_{J\lambda}$ denoted by $S_{J\lambda\delta}$ is responsible for joining of

two deformable cells indexed by λ and δ correspondingly. We assume that this fact is expressed by the relation

$$\mathbf{f}_{I\lambda n} = \mathcal{H}_{\lambda\delta}(\{\mathbf{f}_{I\delta m}\}), \quad (6)$$

where $\mathbf{f}_{I\lambda n}$, $\mathbf{f}_{I\delta m}$ are forces assigned to n -th degree of freedom and m -th degree of freedom within description of λ -th and δ -th deformable cell correspondingly. The mapping $\mathcal{H}_{\lambda\delta}$ expresses structure of joining. In general we can admit to impose some constitutive equations on the mapping $\mathcal{H}_{\lambda\delta}$.

Whole motion of the deformable tissue can be now described by the following equations

$$\Psi_{\lambda i}(\{\mathbf{u}_{f\lambda j}\}, U_{\lambda}) + \mathcal{I}_{\lambda} \ddot{\mathbf{u}}_{\lambda i} = \mathbf{F}_{\lambda i}, \quad (7)$$

where $F = \{\mathbf{F}_{\lambda i}\} = f + f_I$. In this case f represents some external system of forces but f_I are calculated by means of the relation (6) and $\ddot{\mathbf{u}}_{\lambda i}$ is second order time derivative of $\mathbf{u}_{\lambda i}$. Equations given by (7) should be supplemented by the evolution equations

$$\dot{U}_{\lambda} = \mathcal{A}_{U\lambda}(U_{\lambda}, \chi_{\lambda}, \eta_{\lambda}), \quad (8)$$

where \dot{U} is a time derivative of U .

In the last equations we have assumed that subsystems $S_{U\lambda}$ are independent for each $\lambda \in \Lambda_{DC}$. The term "evolution equation" is introduced as similar to evolution equation for internal variables considered in constitutive equations in mechanics of materials. We accentuate by this a similarity with mechanics of materials. However, in this case we have to do with a composite with nonuniform structure. Then, precise theory of structure of this kind should be developed gradually by specification of details of the composite.

Having at our disposal whole tissue we can interpret role of subsystems S_{χ} and S_{SENS} of the deformable cell. The subsystem $S_{\chi\lambda}$ is responsible for generation of an impulse for activation of the subsystem $S_{U\lambda}$. In case of whole tissue we can distinguish a superior over the tissue system S_N which can govern impulses $\{\chi_{\lambda}\}$. Then, subsystems $\{S_{SENS\lambda}\}$ provide to S_N a sensory information by means of variables $r_{SENS\lambda}$ related to states of deformable cells. Action of the system S_N can be expressed symbolically by

$$\chi_{\lambda} = \mathcal{N}_{\lambda}(\{\chi_{\mu}\} \{r_{SENS\nu}\}). \quad (9)$$

The supervising system S_N can apply neural networks for instance, for governing of action of deformable tissue.

5 Discussion of necessity of modelling of deformable cells with the aid of nanoscale and multiscale mechanics

We would say that an idea of the deformable cell which expresses tendency to imitation of muscles is rather simple and well understood intuitively. We can consider relatively simple design criteria associated with the degree of freedom of deformable element with a simple shape composed of a deformable material. However, when we will introduce more advanced requirements, for instance for dynamics of such a structure, then problems of design of such deformable cell can undergo complications. In particular, muscles which are prototype of this idea are extremely complicated when they are considered as a construction. This is so since they satisfy many design criteria related to various scales.

Muscles considered in large scale realize relatively simple function of generation of contractile force and simple deformation. However, at smaller scale, they are highly controllable by chemical reactions. Furthermore, the mechanism of contraction is rather complicated. It rests on synchronized deformation of myosin heads attached to actine which induces sliding of actine fiber with respect to myosin. This, in turn, reflects the design criterion which states that the muscle generates force during contraction. However, when myosin heads are detached from actine the force vanishes but the deformation remains the same. Elongation of the muscle can be induced by an external force. By this we obtain the effect that our hand remains in the position corresponding to moment when muscles are switched off.

Our discussion is aimed at giving the evidence that we have to do with a serious problem considering the deformable cell. At this moment we are not able to solve directly so advanced problems as those related to complexity of muscles. We should elaborate rather a strategy which would allow us to approach gradually to making better and better deformable cells.

In the first step we should explain how we could express design criteria. They can be related to various subsystems of the deformable cell and also to various scales.

We assume that such a strategy consists in developing of a multiscale description within mechanics of materials. Such a description called the collection of dynamical systems with dimensional reduction was introduced in several papers. Let us mention [25,26] for instance. Within such multiscale description nanoscale models are distinguished. This is so since nanoscale approach allows us to model many important mechanisms responsible for inelastic deformation. It enables also cooperation of various models with molecular dynamics in a unified manner. All these facts are essential to defining various, multiscale criteria for design. In par-

ticular, relation to designed structure is closer when we consider smaller scale.

We do not discuss in detail the whole concept of such a multiscale modelling. We introduce here some general framework in order to accentuate role of various scales.

Let us introduce a dynamical system purposed to description of phenomena on the most elementary level called the elementary dynamical system (EDS) given in a general form

$$\dot{\varphi} = L(\varphi, \mathbf{f}) . \quad (10)$$

We introduce a space of solutions $V_T = \{\varphi(t) : t \in T\}$ and also space of forces $\mathcal{F}_T = \{\mathbf{f}(t), t \in T\}$ associated with the Eq. (10) and related to a time interval T .

Let us introduce the operator $\mathcal{L} : V_T \rightarrow \mathcal{F}_T$ constructed with the help of Eq. (10) as $\mathcal{L}(\varphi) = \tilde{\mathcal{L}}(\varphi, \dot{\varphi})$, where $\tilde{\mathcal{L}}$ is obtained from equivalent to (10) equation in the form $\tilde{\mathcal{L}}(\varphi, \dot{\varphi}) = \mathbf{f}$.

Let us introduce also $\bar{V}_T = \{\mathbf{d}(t) : t \in T\}$ and $\bar{\mathcal{F}}_T = \{\bar{\mathbf{f}}(t), t \in T\}$ which are spaces of processes on more averaged level and by this related to larger scale than that one in (10) and also processes associated with forces corresponding to this averaged level of description.

Relation between the two scales are established by mappings $\pi_T : V_T \rightarrow \bar{V}_T$ and also $\pi_{fT} : \mathcal{F}_T \rightarrow \bar{\mathcal{F}}_T$. Let us consider a diagram

$$\begin{array}{ccc} V_T & \xrightarrow{\mathcal{L}_T} & \mathcal{F}_T \\ \pi_T \downarrow & & \downarrow \pi_{fT} \\ \bar{V}_T & \xrightarrow{\bar{\mathcal{L}}_T} & \bar{\mathcal{F}}_T \end{array} \quad (11)$$

Accordingly, the initially introduced equation $\mathcal{L}_T(\varphi(t)) = \mathbf{f}(t)$ induces, owing to assumed π_T and π_{fT} , a dimensionally reduced equation

$$\bar{\mathcal{L}}_T(\mathbf{d}(t)) = \bar{\mathbf{f}} , \quad (12)$$

where $\bar{\mathcal{L}}_T = \pi_{fT} \circ \mathcal{L}_T \circ \pi_T^{-1}$ and the symbol "o" stands for composition of mappings. The operator $\bar{\mathcal{L}}_T$ can be determined with the help of solutions of equation (10) and postulated mappings π_T , π_{fT} for each value of $\mathbf{d}(t)$. In general, such operator is postulated as a skeletal dynamical system SDS (\mathbf{C}) as depending on some constants \mathbf{C} . They can be identified by means of solutions of EDS. In particular EDS can be related to molecular dynamics and SDS (\mathbf{C}) can be related to a continuum theory with finite-dimensional fields. We do not discuss precisely methods of this identification. They are considered in [25,26] for instance.

Let us assume that φ represents variables related to behavior of a material in a small scale. Then, the operator \mathcal{L}_T is determined by means of balance of

mass and energy equations and also by corresponding constitutive equations. In particular it depends on form of the free energy.

The free energy Ψ reflects structure of material. Therefore, this function should take part in the process of design of structures. Let us consider a system of design criteria in relation to a given larger scale by conditions

$$\mathcal{D}_M(\mathbf{d}(t), \bar{\mathbf{f}}, \bar{\mathcal{L}}_T(\bar{\Psi})) \rightarrow \text{inf} \quad (13)$$

and

$$\mathcal{D}_S(\mathbf{d}(t), \bar{\mathbf{f}}, \bar{\mathcal{L}}_T(\bar{\Psi})) \in D_B, \quad (14)$$

where \mathcal{D}_M is a functional which we try to minimize and \mathcal{D}_S is a functional which should have bounds imposed by a set D_B . Functionals \mathcal{D}_M and \mathcal{D}_S represent properties taken into account during the design process. The symbol *inf* denotes the lowest value of the functional which is attainable. Consequently, we see the design process as a kind of optimization problem with imposed constraints.

The variables of functionals \mathcal{D}_M and \mathcal{D}_S can be expressed by means of mappings π_T and π_{fT} and interpretation of (5) in the following form

$$\{\mathbf{d}(t), \bar{\mathbf{f}}, \bar{\mathcal{L}}_T(\bar{\Psi})\} = \{\pi_T(\{\varphi\}), \pi_{fT}(\{\mathbf{f}\}), \pi_{fT} \circ \mathcal{L}_T(\Psi) \circ \pi_T^{-1}\}. \quad (15)$$

When we substitute (15) into (13) and (14) then we obtain a variety of structures represented among others by the smaller scale free energy Ψ which fulfill criteria (13) and (14). In particular, we can minimize (13) to a larger degree having at our disposal a variety of structures corresponding to the smaller scale than those corresponding to the more averaged level.

Let us discuss an example. Let us consider a cubicoid fixed at one end, composed of a shape memory alloy. Then, considering it on a large scale level we can describe its behavior by one generalized coordinate namely a displacement of its end. Then, the internal force Ψ_i in (3) will reflect a behavior of the shape memory alloy with a hysteresis. Let us admit control of such an element by means of an external heat source. In such a case propagation of heat will be rather slow and change of shape should be also slow.

Let us assume a functional $\mathcal{D}_M = T_D$ which represents a time of the deformation between assumed extremal points under a heat flux. We tend towards minimizing this time. Then, efficient supply of heat is of key importance. At larger scale we have a small number of options in order to improve such a heat input. With decreasing of scale we can distinguish more elements and construct more efficient devices.

Within various structures represented by $\{\pi_{fT} \circ \mathcal{L}_T(\Psi) \circ \pi_T^{-1}\}$ we can construct a composite of small wires, for instance, with small parts of external with respect to each wire heat source. Whole system of smaller heat sources is integrated

and is represented by S_U . Thinner elements of SMA have smaller hysteresis and change more easily temperature. Then, the functional T_D can be more minimized considering smaller scale models.

At this moment we encounter the problem of integration of some subsystems of the deformable cell. Some new problems appear when we consider discussed above composite. Integration of subsystems S_D and S_U in such a distributed form needs some additional design criteria related to forms of interactions between distributed subsystems. Thereby, some additional criteria such as (13) and (14) should appear and should be determined for the smaller scale.

Above discussion is aimed at suggesting that the problem of design of deformed cell will have increased complexity together with tendency to improving its performance.

Additional criteria related to smaller scale needs smaller scale models. Let us note that nanoscale models of martensitic transformation [27, 28], plasticity [29], transformation induced plasticity [30] and fracture [31] are formulated having in mind their role in multiscale approach considered above as collection of dynamical systems with dimensional reduction [25]. Whole system of this kind of modelling could be applied in description of deformable cells in relation to various levels of description of their details.

Let us note that investigation of deformable cells in sense described in this paper is related mainly to material sciences. Material sciences are dominated by experimental investigations. Fuel cells are good example, where material sciences down to nanoscale level. However, design of such structures depends mainly on experience of investigators. More precise design needs better theoretical models.

Summarizing, our discussion on multiscale and nanoscale modelling in relation to deformable cells suggests the necessity of further development of these models in order to realize a parallel system of investigation based on both aspects such as theory and experiment. This should, in perspective, improve methods of design of deformable cells.

6 Final remarks

Materials undergoing deformation controlled by various mechanisms and external interactions are frequently applied to manufacturing artificial muscle actuators. Such a possibility is well understood especially when we have intention to mimic muscles or other biological motions. However, efficient application of such materials need more precisely defined conditions in which deformable elements should work.

In this paper we try to give a methodological step towards systemizing various efforts aimed at constructing systems which realize motion similar to that one

provided by muscles. We have defined deformable cell. The first property of such a cell is to realize a simple motion induced by a control parameter. The second property consists in fact that we should consider the deformable cell as a union of subsystems realizing controlling functions as well as ensuring resistance of the cell against damage by external interactions.

Tendency to improving dynamics suggests that deformable cells should be rather miniaturized. This in turn provides a new challenge. All subsystems of the deformable cell should be integrated in small scale which will be probably a task for nanotechnology.

Such a point of view follows in turn increasing role of theoretical descriptions related to nanoscale. By this paper we find motivation for developing of nanoscale models within mechanics of materials viewed as a potential partner for cooperation with experimental investigations.

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