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Problems related to theoretical modelling of production and behavior of thermal barrier coatings

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Abstract

In this paper one discusses the problem of modelling of thermal barrier coatings in an unified way. This approach takes into account both mechanics of materials responsible for behavior of the thermal barrier coatings and its production relying on preparation of material for deposition and the deposition itself. Two pillars of the unified description are considered. The first one is the notion of index of structure. The second one is created by criteria of design of properties of the thermal barrier coatings. It is suggested to apply the multiscale method of modelling for the behavior of material in deposited layer called collection of dynamical systems with dimensional reduction. This multiscale approach is viewed as appropriate theoretical environment for expression of design criteria of the layer. We mean by this the criteria related to mechanical resistance against damage and criteria for thermal properties. It is accentuated that the two-scale segment of multcale modeling composed of molecular dynamics and nanoscale modeling is of primary importance for the design tasks. Possibility of consideration of both mentioned methods of modelling follows from properties of the collection of dynamical system approach which allow us to treat molecular dynamics and continuum mechanics models within one theoretical scheme. Premises for design of production of thermal barrier coatings process are placed in the design of layer properties which could be next transformed into design of indexes of structure corresponding to various stages of the deposition.

Keywords: Thermal barrier coating; Deposition; Multiscale modelling

1 Introduction

Thermal barrier coatings (TBC) are produced to protect elements of constructions against damage induced by high temperature. Thermal barrier coatings are widely applied for protection of turbine blades working at high temperature in

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turbines for propulsion and power generation. The benefit of TBC application in the last case follows from their ability to sustain a high thermal gradient in the presence of sufficient backside cooling. It reduces temperature on the surface of turbine blades composed of superalloy up to approximately 150 °C. The coatings systems applied to turbine blades [26] predominantly consists of partially stabilized zirconia top coat (YSZ), thermally grown oxide (TGO) and a metallic bond coat deposited on superalloy. However, many other materials are investigated with respect to their usefulness to construction of TBC [27]. Thermal barrier coatings are produced usually by a deposition process. The deposition process can be realized by various methods. Let us mention for instance the physical vapour deposition or chemical vapour deposition within a general classification. In the first case the electro spraying method is important and has wide applications [1]. Plasma spraying process [28] or electron beam-physical vapour deposition (EB-PVD) [29] are predominantly applied for production of TBC imposed on turbine blades. The deposition process enables us to produce a layer of material deposited on the previously prepared surface. This region of scientific investigations is dominated by experimentalists which realize in practice various methods of deposition and various means for controlling it. Theoretical descriptions of various kinds are also developed, especially in case of modelling the deposition surface [2–6].

Thermal barrier coating is a considerably smaller object than the turbine blade especially in one dimension. Thus, the problems related to production as well as operation of such a layer differs from traditional engineering objects. Usually, we are not prepared to design of such objects. This is so since the level of design is determined by the level of validity of theory which is applied to description of the designed object. It means that it would be desirable to improve theoretical modelling of thermal barrier coatings in order to extend formal engineering activity to the area of design of such fine objects.

We encounter in literature various approaches to modelling the mechanical properties of thermal barrier coatings. Many papers are devoted to the description of damage of such structures. We are not going to do any review of mechanics related to TBC. Our aim is reduced to make a conclusion why such descriptions should be improved and in what direction it should be done. One considers in literature the cracking of thermal barrier coatings. Elastic and viscoplastic models are applied for description of deformation of material. Finite element methods are predominantly applied. Delamination of layers in TBC is also frequently discussed. Fracture mechanics is applied for functionally graded materials which are also applied for TBC production. Above discussion gives an image on methods which are applied for description of mechanical behavior of TBC. All approaches are directed towards particular aims and use well elaborated methods in mechanics of materials usually applied for considerably larger objects. Scale is taken into

account by division of layers into small parts by finite elements. However, this does not lead to modification of constitutive equations which frequently can depend on scale especially for thin structures and in context of varying temperature. The conclusion is that modelling of processes in TBC layer is rather traditional. However, by further discussion we estimate that such a modelling can be very complex. This is the case for modelling of damage which depend on various mechanisms of inelastic deformation depending on temperature. Therefore, it seems to be necessary to discuss wider context which would provide premises for modelling phenomena in objects which are small at least in one dimension.

The design of thermal barrier coatings should take into account ability of such a structure to protection against the external temperature. However, necessity of operation of TBC layer in thermal cycles when thermal stresses appear, in environment inducing corrosion as well as wearing follows that its resistance against damage is, as a matter of fact, of primary importance. Consequently, design of TBC needs appropriate mechanics of materials for its structure.

Structure of TBC layer depends on the way of its production. The process of production contains both preparation of material for deposition as well as the method of deposition as such. Thereby, we would like to design the layer with respect to properties and its behavior during working but such properties depend just on the structure obtained during the production. It seems that the design process should be concerned with the way of production as well as properties of TBC during its operation. Consequently, the theoretical description should unify both the production process of the layer of material and mechanics of materials related to description of behavior of TBC. Then, the question is, what kind of theoretical description is appropriate for realization of the aim discussed above.

First, we see that fundamental notions of the theoretical description should be associated with preparation of deposited substance and methods of deposition since such processes are responsible just for the kind of material as well as structure which will be obtained within the deposited layer. However, this aspect is not sufficient yet since we have not any aims for preparation of material at this moment. After the deposition we are in fact within the mechanics of materials since we are interested in mechanical, thermal, physical or chemical properties of the obtained layer. Therefore, the second aspect of theoretical description should give a possibility of expression of properties designed for the layer within mechanics of materials. Having at our disposal both mentioned above aspects we have a chance to design the deposited layer and analyse methods of controlling its production within a unified theoretical description. In such a case we could also have a possibility of realization of numerical simulations of processes still before realization of the deposition in practice.

Summarizing, the aim of this paper is to present the concepts which could lead to unification of theoretical description of production and behavior of thermal barrier coatings. The concept discussed here is based on notion of the index of structure and multiscale mechanics of materials. The index of structure is introduced in order to manifest which components of structure are associated with various stages of the preparation as well as realization of the deposition process. Multiscale mechanics of materials is the second pillar of description. It provides theoretical environment for expression of design criteria for the deposited layer.

In this paper one also discusses in a general way problems and physical phenomena which appear especially in ceramic materials constituting TBC layers in order to elucidate complexity of possible theoretical descriptions.

2 On the notion of index of structure

Index of structure is introduced in order to reflect within constructed theory the fact that deposited structure depends on the whole process of preparation of material to spraying, process of spraying and finally the deposition. Let us consider the situation when we prepare a powder for instance. Then, the structure can be characterized by variables describing kind of single crystal contained in subgrains of the powder grain. Thereby, this structure will be present in final deposition layer. Consequently, we should have at our disposal this fact expressed within the theory.

We would say that indexes of structure are related to various stages of the deposition process. However, the term stage can be not sufficiently precise since the stage is in fact related to the time interval in which it occurs. In the deposition process some subprocesses can be carried out in parallel or even can change the order. This is possible since they can happen at various places. Therefore, we introduce the term segment of the deposition process. Thus, preparation of powder is a different segment than spraying which in turn is different than the deposition as such. Within the segments we distinguish processes when indexes of structure depend on time. We assume that the kind of index of structure is the same within the given segment. Taking into account above preliminary discussion we define the index of structure in the following manner:

Definition 2.1 The index of structure related to a segment of deposition process is a set of variables which represents characterization of structure of material which is next transported to the deposition layer.

The term stage can be also applied in what follows. We use them when some segments have to be realized successively and when the context of such a situation

is clear. Let us distinguish some segments corresponding to the deposition process. First the matter should be prepared to spraying. Let it be a powder for instance. Then, the index of structure is related to the form of structure contained in the powder. However, the powder can also be transformed still before spraying. Let us mention nanostructurization for instance [43]. In such a case we would consider several segments during preparation of powder. We distinguish here one segment only for simplicity. As a result we can distinguish the index of structure corresponding to preparation of matter to spraying process. Let it be expressed in the form

$$\mathcal{I}_{PREP} = \{\mathcal{I}_{P1}, \dots, \mathcal{I}_{Pn}\}, \quad (1)$$

where \mathcal{I}_{Pj} stand for various components of index of structure, in particular corresponding to various possible components of powder. We can consider for instance graded material produced during deposition by spraying various components [33].

Let us discuss possible variables which could be components of the index of structure. Let us consider for instance an example which contains variables

$$\mathcal{I}_{Pj} = \{c, g, s_h\}, \quad (2)$$

where group of variables c represents kind of crystal structure of particles in the powder, group of variables g represents size of grains and group of variables s_h reflects shape of grains. We do not discuss variables in more detail at this moment. Let us mention that variables are related to the scale of averaging applied in modelling. Let us note that the free energy Ψ_c related to single crystal grain can be attractive and perhaps very important variable. It characterizes crystal structure similarly as c but contains also additional information on material. In case of c or Ψ_c we have to do with discrete variables since they follows from a finite set of possible crystal structures. Variables of type g or s_h can be continuous. The next segment of deposition process is related to spraying. We assign the index of structure to this process in the following form

$$\mathcal{I}_J = \{\mathcal{I}_{J1}, \dots, \mathcal{I}_{Jn}\}. \quad (3)$$

Let us note that components of \mathcal{I}_J should coincide with \mathcal{I}_{PREP} since spraying does not transform the matter which is sprayed. However, efflux of sprayed matter can be divided into parts in case when various components of powder are sprayed. Then, indexes of structure are also assigned to corresponding parts. It is also admissible that process of spraying has an effect on the structure of sprayed material. The next segment corresponds just to the deposition process as such. Then, the index of structure can be expressed as

$$\mathcal{I}_{DM} = \{\mathcal{I}_S, \mathcal{I}_M\}. \quad (4)$$

The component \mathcal{I}_S stands for the index of structure related to surface of deposited matter. Let us note that form of the surface depends on methods of deposition and by this creates new variables related to the structure. Let us mention for instance local peaks and cavities of the surface which next will be responsible for production of pores in deposited material. Size of such objects and their geometry can be considered as new kind of variables considered as the index of structure. The component \mathcal{I}_M represents structure of three-dimensional deposited material. In this case only the pores are the important elements of structure. Consequently its geometrical characterization can be carried out by means of corresponding index of structure. Role of scale in modelling the deposition, description of evolution of surface of deposited material, and methods of defining of index of structure for deposited material in context of scale, is discussed in [6].

We can also introduce additionally indexes of structure for post-deposition processes. Let them be expressed by

$$\mathcal{I}_{MT} = \{\mathcal{I}_{MT1}, \dots, \mathcal{I}_{MTp}\} . \quad (5)$$

The last step means that we admit various possibilities in changing structure of deposited layer after the deposition process for its improvement.

Let us comment on the role of index of structure in theoretical description of the deposition. Let us mention that when we distinguish some indexes of structure then we are able to observe by theory a path of matter which goes towards the deposition place. Then, it is arguable which part of matter should be placed in a given position and which environment for such a particle of matter should take place.

In case when we use free energy Ψ_c for prepared particle than we are able to discuss also additional, mechanical and physical properties of the deposited matter. All this gives hope that it is possible to design properties of the deposited layer of material together with its production.

3 Discussion of design criteria of the deposited layer

Let us notice that the index of structure corresponding to deposited material is responsible for the form of free energy. Indeed, let us consider for instance the situation where pores are produced in the deposited layer. Then, the density of pores undoubtedly influences the free energy corresponding to the scale applied in modelling of larger structures than size of pores. In case when we are able to control the form of pores then, we control to some degree also the form of free energy. On the other hand this function is of key importance in modelling of mechanical behavior of material. Thereby, we can expect that some criteria for material design can be expressed just by means of free energy.

Above discussion suggests that in order to realize a technological process of production of TBA with required properties we should first create some models of TBC. Such models should have degrees of freedom for a design and should be based on the form of free energy. First we could propose a criterion for the behavior of material in the deposited layer. This criterion would be interpreted as a design. Next taking into account dependence of the free energy on the index of structure we could look for a technology of deposition. Then, the index of structure would be useful since we can modify the deposition process changing just the index of structure.

Let us carry out a general discussion how criteria for design of material layer could be defined. We concentrate our attention on mechanical properties. Then, frequently, strength of the layer is an important property. The strength of layer can be associated with a critical stress for slip in order to accommodate possible change of shape which could happen in another material layer cooperating with the first one during a thermal cycle applied to the system. Critical stresses for crack propagation can also be important. Expression of criteria for material layer design is not simple and immediate in general. This is so since we should first discuss which scale of averaging is appropriate for expression of the criteria. We can have to do with atomic scale. Indeed, during preparation of powder and making various possible dopants we influence arrangement of atoms. In case when we control very precisely atomic arrangement we could be also interested in criteria expressed at atomic level of description. Then, molecular dynamics simulations could have dominant role in expression of mechanical behavior including thermal properties. Usually the deposition process is not so precise. Then, nanoscale level of description can be useful.

Let us discuss possible form of design criteria corresponding to nanoscale. Layer produced by spraying cooperates with material on which this one is deposited. Frequently both materials undergo some thermal cycles. As a result thermal stresses following from various properties of materials can destroy the deposited layer. When we would like to improve this situation we can expect that both materials can be chosen in order to have the same thermal strains or similar ones when they are considered separately. If it would not be possible then in order to avoid fracture of the deposited layer we would like to have property expressed by possibility of stress relaxation in the layer by slips or other forms of inelastic deformation in material. Summarizing we see that critical values of stresses for slip initiation or crack propagation can play very important role in the design of deposited layer. In nanoscale model of plasticity [7, 9] we assume that slip is initiated when stress considered in a slip system attains a critical value expressed by

$$\tau = \tau^* . \quad (6)$$

Similarly, the crack propagates within the nanoscale model of fracture [8,9] when critical stress in a fracture system

$$\sigma = \sigma^* . \quad (7)$$

attains a corresponding critical value.

Structure of slip is defined by slip systems $\{\mathbf{m}_i, \mathbf{n}_i\}$, where \mathbf{m}_i indicates direction of slip and \mathbf{n}_i is perpendicular to the surface of slip. Slip surfaces are considered as discontinuity surfaces for displacements where deformation by slip is continued. Thus, beyond the slip surfaces the material is nonlinearly elastic. Let us note that slip systems as well as fracture systems are expressed within the nanoscale model by means of free energy [7,9].

Let us distinguish also the stress σ_∂ in a vicinity of boundary of the deposited layer where the contact with another material is realized. Within this symbolic notation we can interpret σ_∂ also as a surface force associated with the contact between layers. Thus, σ_∂ is interpreted here as one symbol for various mathematical objects for simplicity.

We can discuss design of the deposited layer corresponding to nanoscale modelling within the set of conditions

$$|\sigma_\partial| \rightarrow \min , \quad (8)$$

$$\tau^* \in [\tau_a, \tau_b] \quad (9)$$

or

$$\tau^* \rightarrow \max , \quad (10)$$

$$\tau^*(\Psi) <_{GB} \sigma^*(\Psi) , \quad (11)$$

$$\sigma^* \rightarrow \max , \quad (12)$$

$$\{\mathbf{m}_i, \mathbf{n}_i\}(\Psi) = \Phi , \quad (13)$$

where Φ is a given function. The condition (8) leads to decreasing of stresses in the region where contact between various materials takes place. The condition (9) can be useful for design of possibility of stress relaxation in case when various material layers interact. This perhaps should be considered together with Eq. (11), where the relation $<_{GB}$ means that $\tau^*(\Psi)$ goes before $\sigma^*(\Psi)$. We have accentuated here dependence of both stresses on the form of free energy Ψ since slip systems and fracture systems are defined just in terms of this function. The condition (11) can be interpreted as a criterion for ductility. Thus by Eq. (11) we express tendency to preferring first slip before crack.

Sometimes we could be interested directly in property (10) together with the condition (12). Having at our disposal slip systems expressed by means of the

free energy we could influence also the structure of slips by option of appropriate dopants and changing in such way the \mathcal{I}_{PREP} . It affects the form of Ψ . Then, the given function Φ in the condition (13) expresses our expectations on the kind of admissible slip systems in connection with the index of structure. Let us note that in nanoscale models we use free energy for defining all critical conditions. Then, such conditions are expressed by critical strains directly but intermediately only by critical stresses. In above discussion we use stresses for making interpretation of our intentions more clear.

Modelling at a larger scale of averaging leads to another description. Let us mention the crystal plasticity [11, 12], which is designed to modelling plastic phenomena in a single crystal with scale of averaging related to micrometers. Then, slip systems are also distinguished. Plastic deformation is described by the strain tensor. However, slip bands can be modelled as motion associated with the discontinuity surface. The design criteria can be associated with critical value of stresses expressed in slip systems in similar manner as this was considered above for nanoscale models by

$$\tau^* \in [\tau_a, \tau_b] . \quad (14)$$

Furthermore, we can be interested how small cracks develop when the slip is continued. We can expect that slip within slip bands is not perfect. It means that some instabilities in flow lead to breaking of interatomic bonds on slip surfaces. Then, evolution of cracks within slip bands is much more probable than in other regions of material. In order to describe evolution of such cracks we can introduce some internal state variables. Let us consider for instance the variable

$$\xi_{CR} = \frac{S_{CR}}{S_{SL}} , \quad (15)$$

where S_{CR} is a surface measure of cracks referred to measure S_{SL} of amount of whole slip surfaces contained in the slip band. Then, evolution of this variable can be described by means of the evolution equation

$$\dot{\xi}_{CR} = A_{CR}(h) , \quad (16)$$

where h represents all variables applied within this model.

We are interested to possible degree on slowing down of development of cracks in the slip band. Consequently, we can postulate a criterion

$$\left| \frac{\partial A_{CR}}{\partial h} \right| \rightarrow \min , \quad (17)$$

where we consider the length of vector of derivative of the function A_{CR} as a measure of velocity of changes which we would like to decrease.

Let us note that we have to do with an open problem how precisely the evolution equation (16) should be determined. However, its form depends on structure of deposited material and by this on the index of structure. Hitherto we have discussed descriptions in a single crystal. However, a part of index of structure describes porous structure and other features which are created by the deposition process. Thereby, we should discuss also more averaged descriptions related to scale of averaging larger than size of pores.

We have to do with several possibilities. Perhaps structure produced by deposition enables us discriminating some slip systems with the aid of the free energy in a similar manner as this is done for nanoscale level of description but in case of more averaged medium. Then, we can consider similar criteria for material design as those discussed by means of Eqs. (16) and (17).

If the averaged medium is more homogeneous we can apply plasticity related to still larger scale of averaging. It is preferable to apply approaches using free energy and internal state variables as this is done in [13,14] for instance. Option of such an approach is motivated by relations between the free energy and index of structure and following from this fact unified theoretical description of deposition process and mechanical properties of the layer.

Above discussion is devoted to accentuating role of methods of modelling in determination of possible criteria for design of deposition layers. It seems that multiscale aspect of modelling is of great importance. This is so when we would like to describe particular mechanisms of inelastic deformation which in turn can be of key importance for correct working of thermal barrier coatings.

4 Structural and physical properties of pure zirconia and partially stabilized zirconia

We have discussed above some general aspects associated with mathematical description and design of deposited layers. By this discussion we tend to develop gradually views on method of modelling of deposition process and deposited layers. Furthermore, doing this we try to promote particular category of deposited layer, namely we would like to accentuate validity of thermal barrier coatings. Validity is related to their technical applications. Furthermore, complex phenomena in thermal barrier coatings provide also motivations for development of multiscale mechanics of materials us such. Consequently, by above discussion we would like to obtain also some justification why multiscale and especially nanoscale mechanics of materials should be developed in the context of thermal barrier coatings production and modelling.

In order to indicate such reasons we discuss processes in zirconia which is an important material for building just thermal barrier coatings. Complexity of

phenomena in zirconia and zirconia based mixtures as well as multiphase composites shows that simple and very averaging approach by traditional continuum mechanics approach perhaps is not sufficient. The question which approach would be appropriate for such material, especially placed in layers, leads to some conclusions developed in the next part of this paper. Zirconia (ZrO_2) crystal structure changes with temperature. At atmospheric pressure it transforms from cubic crystal lattice into tetragonal one for 2200 °C. Next with decreasing of temperature it can be transformed into monoclinic crystal structure for 1150 °C [15].

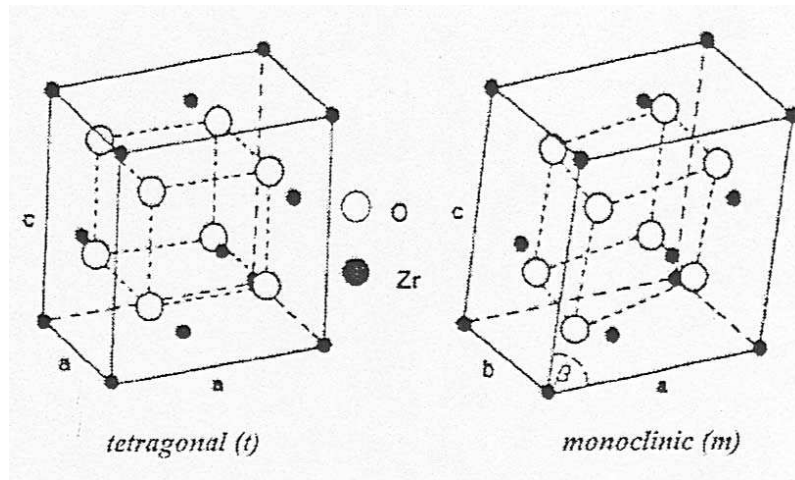


Figure 1. Change of distribution of atoms in ZrO_2 during tetragonal to monoclinic transformation.

In the last case we have to do with martensitic transformation. Changes in distribution of atoms during the transformation $t \rightarrow m$ are shown in Fig. 1. Possible orientations of monoclinic structure with respect to tetragonal one are shown in Fig. 2 following from [16]. In Figs. 3 and 4 we show how various variants of martensite of zirconia accommodate within parent phase and create by this microstructure. Above illustrations allow us to imagine complexity of martensitic transformation. Various orientations are associated with various placements of habit planes in parent phase. This induces various kinds of rotations of separate martensite variants.

Transformation of pure zirconia from tetragonal to monoclinic phase induce large volume changes which can induce fracture. As a result of this the material is not too convenient for applications. However, the addition of oxides such as CaO , MgO or Y_2O_5 reduce the m -phase and stabilize tetragonal phase (partial stabilization) at the same temperature. Such material is frequently called the partially stabilized zirconia (PSZ). With increasing of amount of dopants we can stabilize also the cubic phase (full stabilization) [17].

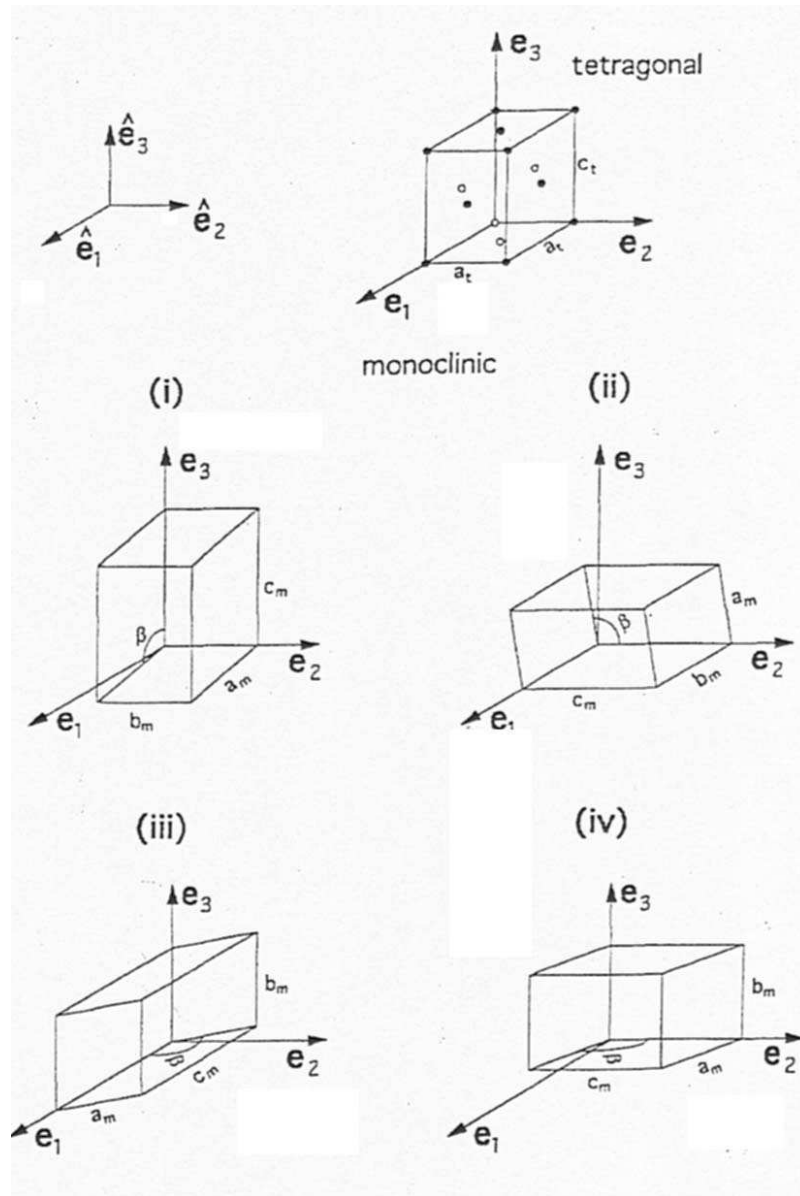


Figure 2. Various orientations of monoclinic structure with respect to tetragonal one in ZrO_2 .

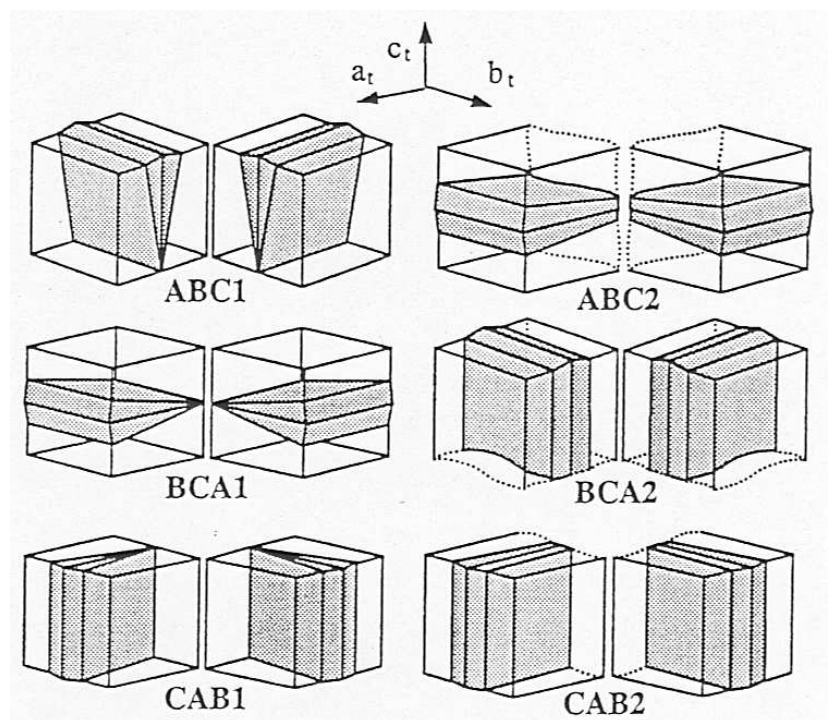


Figure 3. Selfaccommodating martensite variants in ZrO_2 .

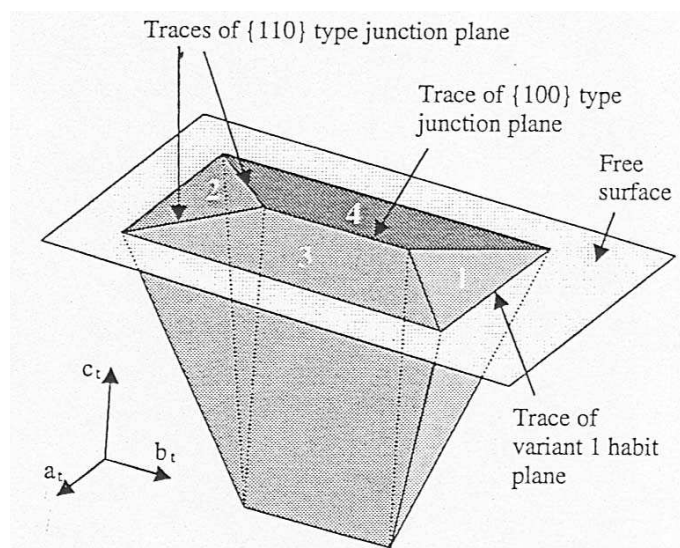


Figure 4. An example of martensitic structure in ZrO_2 .

Interesting mechanical properties appear when the grains in tetragonal phase are metastable [18]. Such a situation happens when grains containing low concentration of yttria are placed within matrix with high concentration of yttria. Then, stress induced martensitic transformation is possible. This phenomenon is associated with transformation strengthening [19].

Possibility of transformation of stabilized metastable tetragonal phase grains placed in cubic phase by stress makes more difficult propagation of crack. Indeed, when plastic zone near the tip of the crack is created then, large stresses produced there can transform the tetragonal phase into monoclinic one. This changes distribution of stresses in vicinity of the tip of the crack. When structure and distribution of grains is appropriate than the change of stresses makes propagation of the crack impossible. It means that larger external stress has to be applied in order to activate fracture. As a result strengthening of material increases what makes this form of zirconia more applicable. Above discussed property can be attained at low temperatures. Such a situation is shown in Fig. 5 [19]. Let us mention that doped with yttria fine grained zirconia polycrystal have also interesting mechanical properties for larger temperatures. It exhibits structural superplasticity [18,20,21]. This effect can be useful in applications in many technological processes. Let us note however, that inclination to superplasticity can also be convenient in relaxation of stresses when the material cooperates with another one in a kind of composite for instance.

Above concise discussion shows that inelastic deformation of partially stabilized zirconia has various mechanisms. First, the martensitic transformation appears as transformation from tetragonal to monoclinic crystal structure. Furthermore, we can admit also slips as mechanism of inelastic deformation in some temperature range and applied external stresses [22,23]. In case when PSZ is considered as a kind of composite, considering grains of tetragonal phase within cubic phase then the stress induced transformation in grains can be considered. When, we apply such a situation to crack tip zone then processes are rather complicated. Inclination to superplasticity can also be important in some temperature range. Let us mention that we have an intention to apply this material in thermal barrier coatings where cycles of temperature are rather frequent. Then, the mechanisms of deformation associated with processes near to boundary of grains can be important.

Creation of microstructure related to martensite, especially in thin layers, needs careful modelling. It seems that nonoscale models of martensitic transformation are appropriate to this end. Such models have been constructed for copper based alloys in [9,24]. Possible cooperation of slip plasticity and martensitic transformation at nanoscale level of description has been discussed in [9,25]. This approach could also be developed towards application in ceramics. Nanoscale

models are convenient to cooperation with molecular dynamics methods. In above discussion we see that temperature has important influence on quality of processes and change of mechanisms of inelastic deformation. In general it seems that application of molecular dynamics is inevitable in order to support nanoscale models and explain finer processes. Therefore, above discussion supports the point of view that mechanical models applied in modelling of complex processes in small scale, such as those ones in PSZ for instance, should be realized on the way which gives a chance in a perspective, for cooperation of introduced models just with the molecular dynamics method.

5 Thermal barrier coatings

Thermal barrier coatings (TBC) are produced in order to protect chosen parts of constructions against high temperature. Usually they have multilayer structure and lower temperature on protected surface in case of additional cooling of this surface.

Thermal coating systems can be applied to turbine blades [26]. Usually they consist of partially stabilized zirconia top coat (YSZ), thermally grown oxide (TGO) and a metallic bond coat deposited on surface of turbine blade composed of superalloy. Many other materials are also investigated with respect to their potential application to construction of TBC [27]. TBC applied to turbine blades allow us to reduce temperature on the surface of superalloy up to approximately 150 °C. In the last case thermal barrier coatings are produced usually by deposition process with the aid of plasma spraying process [28] or electron beam-physical vapour deposition (EB-PVD) [29].

Thermal properties of TBC are mainly represented by a layer of Y-PSZ which has convenient thermal strains and is able to reduce stresses, in case of presence of various layers, induced during thermal cycles. However, the PSZ is transparent to oxygen, As a result thermally grown oxide (TGO) is produced between top coat built of partially stabilized zirconia and bond coat. TGO is composed of Al_2O_3 . The bond coat is the reservoir of Al for production of TGO. As a result TGO increases and its structure changes during working. Thermal strains in TGO layer are not well fitting to other layers of the thermal barrier. Therefore stresses generated by the growing layer lead with time to damage of the thermal barrier.

Various challenges are associated to the design of TBC. We can try to control TGO. This is however difficult. Therefore we can try to reduce influx of oxygen into the region of bond coat by application of various methods of surface modification. Let us mention high-intensity pulsed ion beam (HIPIB) [30] or laser treatment of surface of TBC [31,32]. Above methods lead to melting of surface of thermal barrier coatings and by this introduce modification of its structure. As a result

influx of oxygen into bond coat within TBC can be reduced. Improving of TBC properties against oxidation can also be attained by production of graded coatings. Graded transition of concentration from Al_2O_3 to YPSZ leads to obtaining good thermal insulation of stabilized zirconia with low oxygen diffusivity [33,34].

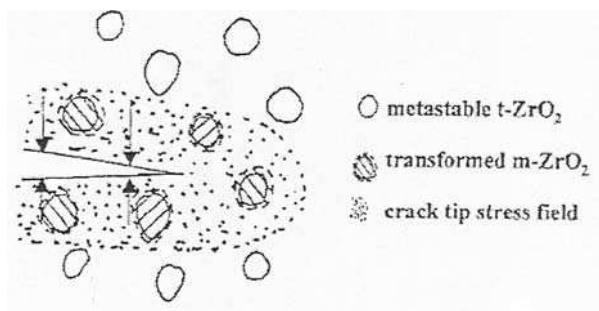


Figure 5. Propagation of crack in matrix with tetragonal, metastable grains of YPSZ.

Graded materials can also reduce thermal stresses owing to gradual transition between layers of various properties. Graded thermal barrier coatings can be more resistant to damage than non graded ones [35]. Thermal properties of TBC can be modified by decreasing thermal conductivity within the layer structure or by improving reflexivity of thermal radiation. This can be attained by adding some dopants into the layer [36] or by controlling of structure of pores, eg by producing zig-zag pore microstructure [37]. Widely applied method of improving thermal insulation for TBC is creating its multilayer structure [36,38].

Summarizing, we see from the above discussion that thermal barrier coating are rather complex objects in small scale and have various functions assigned to various elements of this structure. In particular important properties are associated with thermal properties. However, good thermal properties are not sufficient for correct work of TBC since the layers have to be stable in conditions frequently extremal with respect to stresses. Thus, both thermal properties and mechanical properties have to be the aim in design of thermal barrier coatings.

The deposition process complicates additionally the structure of thermal barrier coatings. We obtain usually a porous structure during the deposition. Furthermore, we produce frequently nonhomogeneous distribution of components intentionally. Let us mention the graded coatings for instance. On the other hand we have discussed previously phenomena in zirconia and partially stabilized zirconia which are estimated as complex. Therefore, an additional complication of structure by introduction of pores or composite character of the layer makes modelling of thermal barrier coatings still more complicated.

6 Remarks on multiscale modelling in mechanics of materials

6.1 General framework

Previous discussion shows that thermal barrier coatings are structures in which complex phenomena in material can happen. Furthermore they are burdened with responsibility for fulfilling various functions ensuring resistance and safety of coated construction. Mechanisms governing behaviour of such layers are frequently related to very small scale or even need analysis associated with atomistic scale. Thereby, in order to take into account whole phenomena in TBC and to have the possibility of expression of design criteria we should consider a mathematical description for mechanics of materials related to various scales.

Small scale behavior of materials leads to increasing role of dynamics of processes in comparison with larger scale models. In particular, the most complex dynamics is related to atomistic scale where we usually apply molecular dynamics methods. All this suggests that methods of modelling should take into account formalization of the scale of averaging of processes and a dynamical system approach. Such kind of modelling has been introduced and discussed in papers [9, 10, 42] and is called the collection of dynamical systems with dimensional reduction. We discuss here concisely just this method of modelling.

Our discussion is related first to two-scale modelling in an abstract form. We consider the most elementary model as a foundation for determining by means of it a more averaged and simpler model. Consequently, we introduce a dynamical system aimed at description of phenomena on the most elementary level. Such a system called further the elementary dynamical system (*EDS*) is given in a general form

$$\dot{\varphi} = L(\varphi, \mathbf{f}), \quad (18)$$

where $\varphi \in \mathcal{M}_\varphi$ is the variable of this system, \mathcal{M}_φ is a space of admissible values of this variable, $\mathbf{f} \in \mathcal{F}$ represents external interactions acting on this system and \mathcal{F} stands for space of admissible values of \mathbf{f} .

External interactions are not always expressed in relative simple form given by \mathbf{f} . They can also appear as interactions with other dynamical systems. Therefore, we introduce also an extended dynamical system

$$\dot{\varphi}^r = L(\varphi^r, \mathbf{f}^r), \quad (19)$$

where $\varphi^r = \{\varphi, \varphi^e\} \in \mathcal{M}_{\varphi^r}$ and $\mathbf{f}^r = \{\mathbf{f}, \mathbf{f}^e\} \in \mathcal{F}_r$. In other words the dynamical system (18) is a part of that one defined by (19) and can be viewed as a particular case of (19). As a result an external dynamical system with variable φ^e can be additionally distinguished, as a source of external interactions acting on *EDS*.

This gives a possibility of discussing larger class of interactions of (18) with an external world.

The dynamical system Eq. (18) describes more elementary processes and its form is, by assumption, the most complex. We tend towards simplifications of this system. To this end we introduce a partition of Eq. (18) into a collection of P dynamical systems. This is carried out by partition of variable $\varphi = \{\varphi_h\}$, $h \in I_P = \{1, 2, \dots, P\}$.

In order to use this partition for further simplifications we introduce also additional notations, sets and mappings. Let $\prod_h \mathcal{M}_h$ be Cartesian product of sets \mathcal{M}_h , where \mathcal{M}_h stands for the set of admissible values of $\{\varphi_h\}$. Let us introduce $\mathcal{M}_\Pi \subset \prod_h \mathcal{M}_h$ as a subset of the Cartesian product. Then, \mathcal{M}_Π consists of $\varphi = \{\varphi_h\}$ which are possible solutions of Eq. (18). We consider also a projection $\pi_h : \mathcal{M}_\Pi \rightarrow \mathcal{M}_h$ in the Cartesian product.

Let us distinguish also a collection of dynamical systems for the extended system and a set of indexes I_R related to them. Then, $I_R = I_P \cup I_E$, $I_P \cap I_E = \emptyset$, where I_P is related to (18) and $I_E = I_R - I_P$ is connected with the external system. Furthermore we distinguish a group of dynamical subsystems $I_G \subset I_P$ by selection of corresponding indexes. Then, $I_O = I_R - I_G$ represents indexes defining external with respect to I_G dynamical subsystems within (19).

New simplified equations have to be based on balance of mass and energy equations as the most fundamental physical laws for mechanics of materials. In order to create such equations for the collection of dynamical systems we should have at our disposal a set of additional notions making possible to formulate them. Therefore we introduce the following assumptions which represent general properties of the collection of dynamical systems distinguished within the elementary dynamical system:

1. Subsystems are distinguished by determination of groups of variables $\varphi_h = \{\varphi_{h\alpha}\}$, where $\alpha \in I_{Ah}$, I_{Ah} is a finite set related to separate h -th subsystem and $h \in I_P$.
2. There exists a function $\tilde{m}_h(\varphi_h) = \{m_{h1}, \dots, m_{h\beta_h}\}$ which assigns a set of masses for h -th subsystem. The total mass of the system is $m_h = \sum_i m_{hi}$. We have also that $\sum_h \beta_h = N$, where N is the total number of masses. Then, the functions $\tilde{m} : \mathcal{M}_\Pi \rightarrow R^P$ with property $\pi_h \circ \tilde{m}(\{\varphi_h\}) = m_h$ and $m : \mathcal{M}_\Pi \rightarrow R$, $m(\{\varphi_h\}) = \sum m_h$ determine the total mass related to each subsystem and the total mass related to (18) respectively.
3. There exists a function $\tilde{E} : \mathcal{M}_\Pi \rightarrow R^P$, $\pi_h \circ \tilde{E}(\{\varphi_h\}) = E_h$ which assigns a value of energy to each of subsystems and $E : \mathcal{M}_\Pi \rightarrow R$, $E(\{\varphi_h\}) = \sum_h E_h$ determines the total energy related to (18).

4. There exists a family of mappings $J_{ij} : \mathcal{M}_{\Pi} \rightarrow R$, $i, j \in I_P$, $J_{ij}(\{\varphi_h\}) = J_{ij}$ called flux of mass from j -th subsystem to i -th subsystem and $J_{ij} + J_{ji} = 0$, $J_{ii} = 0$.
5. There exists a family of mappings $W_{ij} : \mathcal{M}_{\Pi} \rightarrow R$, $i, j \in I_P$, $W_{ij}(\{\varphi_h\}) = W_{ij}$ called the flux of energy from j -th subsystem to i -th subsystem and $W_{ij} + W_{ji} = 0$, $W_{ii} = 0$.
6. Source of mass is determined by the function $c : \mathcal{M}_{\Pi} \rightarrow R^P$, $c(\{\varphi_h\}) = \{c_i\}$. Then, $c_i = \pi_i \circ c(\{\varphi_h\})$ can be considered for each subsystem of the whole system and stands for the source of mass in i -th subsystem.
7. Source of energy is determined by the function $R : \mathcal{M}_{\Pi} \rightarrow R^P$, $R(\{\varphi_h\}) = \{R_i\}$. Then, $R_i = \pi_i \circ R(\{\varphi_h\})$ can be considered for each subsystem of the whole system and stands for the source of energy in i -th subsystem.
8. Geometrical objects can be assigned to each subsystem. This is carried out with the help of mappings $G_x : \mathcal{M}_{\Pi} \rightarrow E_e^P$, $G_L : \mathcal{M}_{\Pi} \rightarrow (2^{E_e})^P$, $G_S : \mathcal{M}_{\Pi} \rightarrow (2^{E_e})^P$, $G_V : \mathcal{M}_{\Pi} \rightarrow (2^{E_e})^P$, where E_e is the Euclidean space. The map G_x assigns some distinguished points to subsystems, G_L introduces one-dimensional, G_S two-dimensional, G_V three-dimensional geometrical objects considered as subsets of E_e and accompanied by distinguished subsystems.
9. Position vectors $\mathbf{q} = \{\mathbf{q}_{h1}, \dots, \mathbf{q}_{h\beta_h} : h \in I_P\}$ can be introduced by means of mapping P_q . $Q = \{\{\mathbf{q}_{h1}, \dots, \mathbf{q}_{h\beta_h}\}\}$, $\dim Q < \infty$, $P_q : \mathcal{M}_{\varphi} \rightarrow Q$, $P_q(\varphi) = \mathbf{q}$. All discussed assumptions and functions can also be introduced for the extended dynamical system (19).

Above assumptions enable us to discuss various notions associated with possible simplifications related to elementary dynamical system. In particular geometrical object can create relation between *EDS* and space in which the dynamical system acts. They can assign a volume of space occupied by a dynamical subsystem for instance. This can lead to various approximations with the help of geometry and introducing continuum for instance.

With the help of above assumptions we are able to carry out analysis of interchange of mass between subsystems as well as to consider possible sources of mass which appear within subsystems. Let us consider an arbitrary part of *EDS* defined by $I_G \subset I_P$. Let I_O define the external with respect to I_G dynamical system. Then, we are able also to express the balance of mass equation for collection of dynamical systems in the following form

$$\sum_{i \in I_G} (\dot{m}_i - c_i) + \sum_{i, j \in I_G} J_{ij} + \sum_{i \in I_G, j \in I_O} (J_{ij} + J_{ji}) + \sum_{i, j \in I_O} J_{ij} + \sum_{i \in I_O} (\dot{m}_i - c_i) = 0. \quad (20)$$

Sum of masses interchanged between subsystems within I_G without any interchange with an external subsystems is equal to zero. Thus, we have $\sum_{i,j \in I_G} J_{ij} = 0$.

As a result we can express the balance of mass equation connected with the group of subsystems represented by I_G with the help of formula

$$\sum_{i \in I_G} (\dot{m}_i - c_i + \sum_{j \in I_O} J_{ij}) = 0 . \quad (21)$$

In equation (21) the terms J_{ij} describing interchange of mass with external system I_O appear. Then, the equation (21) is not entirely determined. Therefore we should introduce an additional condition

$$J_{ij} = \bar{J}_{ij} , j \in I_O . \quad (22)$$

The external efflux \bar{J}_{ij} should be postulated by a kind of constitutive equations or can be defined by evolution of the dynamical system defined by means of I_O .

The balance of energy equation has a similar structure as the balance of mass equation and is given by

$$\sum_{i \in I_G} (\dot{E}_i - R_i) + \sum_{i \in I_G, j \in I_O} (W_{ij} + W_{ji}) + \sum_{i \in I_O} (\dot{E}_i - R_i) = 0 . \quad (23)$$

The balance of energy equation for group of subsystems I_G interacting with groups of subsystems I_O , is given by

$$\sum_{i \in I_G} (\dot{E}_i - R_i + \sum_{j \in I_O} W_{ij}) = 0 \quad (24)$$

with additional conditions

$$W_{ij} = \bar{W}_{ij} , j \in I_O . \quad (25)$$

Equations (21), (22) and (24), (25) represent a general form of balance of mass and energy equations related to arbitrary distinguished group of subsystems within the collection of dynamical systems and can be premises for further considerations.

6.2 Dimensional reduction procedure

Dimensional reduction procedure is introduced in order to carry out transition from elementary dynamical system to the more simple one which describes chosen properties of *EDS* in an averaged manner. Thereby, the simpler dynamical system represents the more averaged level of description in comparison to *EDS*.

In the first step of the dimensional reduction we select new variables appropriate for description after averaging. Let $\mathbf{d} = \{\mathbf{d}_h\}$, $h \in I_R$ be a set of new

variables which allows us to describe, approximately, physical states represented by miscellaneous φ^r considered as solutions of an extended elementary dynamical system. Let $\bar{\mathcal{M}}$ stands for space of admissible values of \mathbf{d} . The variable \mathbf{d}_h is designed to describe behaviour of h -th subsystem in a simplified form. The index h is related to previously discussed division of elementary dynamical system into subsystems. Thereby, the division represented by set I_R is related to both *EDS* and an averaged dynamical system obtained after application the dimensional reduction procedure. By assumption we have that $\dim \bar{\mathcal{M}}$ is considerably smaller than $\dim \mathcal{M}_\varphi$ owing to applied averaging.

Let $V_T = \{\varphi(t) : t \in T\}$, $V_{Tr} = \{\varphi^r(t) : t \in T\}$ and $\bar{V}_T = \{\mathbf{d}(t) : t \in T\}$. Introduced spaces represent processes described by *EDS* an extended *EDS* and averaged dynamical system. The first element of the dimensional reduction procedure is based on introduction of a mapping $\pi_T : V_{Tr} \rightarrow \bar{V}_T$ which assigns dimensionally reduced process $\mathbf{d}(t)$ to $\varphi^r(t)$ on the time interval T . We introduce also $\mathcal{F}_T = \{\mathbf{f}(t), t \in T\}$ and $\bar{\mathcal{F}}_T = \{\bar{\mathbf{f}}(t), t \in T\}$ with mapping $\pi_{fT} : \mathcal{F}_T \rightarrow \bar{\mathcal{F}}_T$ which transform force processes between elementary and reduced system. We can discriminate parts $\mathbf{d}^p(t)$ and $\mathbf{d}^e(t)$ related to *EDS* and external dynamical system within the process $\mathbf{d}(t)$. Similar partition is possible for $\mathbf{f}(t)$ and $\bar{\mathbf{f}}(t)$ since they are considered here for extended system. Thus, we carry out the dimensional reduction for the extended dynamical system (19). However, our interest is related mainly to *EDS* given by (18).

Let us introduce an operator $\mathcal{L} : \tilde{\mathcal{L}}(\varphi, \dot{\varphi})$ where $\tilde{\mathcal{L}}$ is obtained from equivalent to (19) equation in the form $\tilde{\mathcal{L}}(\varphi, \dot{\varphi}) = \mathbf{f}^r$. By this we assume also that such a reformulation is possible. Then, the operator acting on processes $\mathcal{L}_T : V_{Tr} \rightarrow \bar{\mathcal{F}}_T$ is induced directly by means of \mathcal{L} for each $t \in T$. Let us consider a diagram

$$\begin{array}{ccc}
 V_{Tr} & \xrightarrow{\mathcal{L}_T} & \mathcal{F}_T \\
 \pi_T \downarrow & & \downarrow \pi_{fT} \\
 \bar{V}_T & \xrightarrow{\bar{\mathcal{L}}_T} & \bar{\mathcal{F}}_T
 \end{array}
 \tag{26}$$

Consequently, the initially introduced equation $\mathcal{L}_T(\varphi(t)) = \mathbf{f}(t)$ at the *EDS* level induces, owing to introduced mappings π_T and π_{fT} , a dimensionally reduced equation

$$\bar{\mathcal{L}}_T(\mathbf{d}(t)) = \bar{\mathbf{f}},
 \tag{27}$$

where $\bar{\mathcal{L}}_T = \pi_{fT} \circ \mathcal{L}_T \circ \pi_T^{-1}$. The operator $\bar{\mathcal{L}}_T$ can be determined with the help of solutions of equation (19) and postulated mappings π_T , π_{fT} for each value of $\mathbf{d}(t)$

obtained with the aid of mapping π_T . However, structure of the operator $\bar{\mathcal{L}}_T$ is not discussed yet since too small number of assumptions is done at this moment.

Let us discuss a similar diagram for a group of subsystems $I_G \subset I_P$. Then, we carry out the following decomposition $V_{Tr} = V_{TG} \times V_{TO} = \{\varphi(t) = \{\varphi_g(t), \varphi_l(t)\}, g \in I_G, l \in I_O\}$. We introduce also decomposition $\mathcal{F}_T = \mathcal{F}_{TG} \times \mathcal{F}_{TO}$ in a similar way. Above decompositions of domain and range leads to expression of the form of operator \mathcal{L}_T by $\mathcal{L}_T = \mathcal{L}_{T(\varphi_l)}(\{\varphi_g(t)\}) \times \mathcal{L}_{T(\varphi_g)}(\{\varphi_l(t)\})$. The operator $\mathcal{L}_{T(\varphi_l)} : V_{TG} \rightarrow \mathcal{F}_{TG}$ depends on φ_l . Usually, not all $\varphi_l \in V_{TO}$ are necessary for determination $\mathcal{L}_{T(\varphi_l)}$.

Let I_{GO} stands for a set of indexes which indicate variables necessary for determination of the operator $\mathcal{L}_{TG} := \mathcal{L}_{T(\varphi_l)}$. Then, the operator \mathcal{L}_T can be expressed in a simplified form as $\mathcal{L}_{TG} \times T_C$, where $T_C = T_C(\varphi_g, \varphi_c)$, $c \in I_{GO}$. With the help of T_C we are able to introduce additional equations necessary for determination of φ_c defining form of \mathcal{L}_{TG} within \mathcal{L}_T . The space V_{Tr} is reduced to $V_{TG} \times V_{TC}$ in this case.

The diagram (26) with application of decompositions discussed above can be expressed now in the following form

$$\begin{array}{ccc}
 V_{TG} \times V_{TC} & \xrightarrow{\mathcal{L}_{TG} \times T_C} & \mathcal{F}_{TG} \times \mathcal{F}_{TC} \\
 \pi_T \downarrow & & \downarrow \pi_{fT} \quad \downarrow \pi_{fTC} \\
 \bar{V}_{TG} \times \bar{V}_{TC} & \xrightarrow{\bar{\mathcal{L}}_{TG} \times \bar{T}_C} & \bar{\mathcal{F}}_{TG} \times \bar{\mathcal{F}}_{TC} .
 \end{array} \tag{28}$$

Accordingly, the dimensionally reduced equation describing evolution of a group of subsystems is given by

$$\bar{\mathcal{L}}_{TG(\mathbf{d}_c)}(\{\mathbf{d}_g(t)\}) = \{\bar{\mathbf{f}}_g\}, \tag{29}$$

$$\bar{T}_{C_c}(\mathbf{d}_g(t), \mathbf{d}_c(t)) = \mathcal{B}_c. \tag{30}$$

Decomposition of the operator \mathcal{L}_T is carried out in order to accentuate separately the behavior of *EDS* and the reduced *EDS* as associated with part representing external interactions. In case of continuum mechanics, for instance, such a decomposition can be associated also with boundary conditions.

Diagram (28) allows us to solve Eqs. (29) and (30) by means of solutions of Eq. (19) and postulated form of π_T , π_{fT} , π_{fTC} . However, we would like to have a precise structure of $\bar{\mathcal{L}}_{TG}$ and \bar{T}_C in order to have at our disposal dimensionally reduced equations possible for solving, without using Eq. (19) incessantly. Obtaining of such equations is possible by means of postulating of the skeletal

dynamical system $SDS(\mathbf{C})$ which depends on the family of constants \mathbf{C} . The role of SDS is to represent a larger class of systems which encompass approximately Eqs. (29), (30). Accordingly, the general form of SDS taking into account Eqs. (29), (30), can be expressed as

$$\{\bar{\mathcal{L}}_{TG}, \bar{T}_C\}(\mathbf{C})(\mathbf{d}_g, \mathbf{d}_c) = \{\bar{\mathbf{f}}, \mathcal{B}\}. \quad (31)$$

Then, with the help of the identification method, we determine $\mathbf{C} = \bar{\mathbf{C}}$ and, as a result, a reduced dynamical system $RDS = SDS(\bar{\mathbf{C}})$. Finally, RDS represents an approximation of Eqs. (29) and (30).

Previous discussion of balance of mass and energy equations in relation to the elementary dynamical system divided into subsystems and above decomposition of operators into qualitatively various parts provides premisses for determination of the form of SDS . Let us mention that since balance of mass should be satisfied, we obtain that masses related to dynamical system also undergo dimensional reduction. This is introduced by additional mapping $\pi_M(\{m_{hi}\}) = \{M_{hp}\}$. Consequently, M_{hp} are inertia coefficients related to h -th subsystem and should be present in the postulated form of SDS .

Efficiency of dimensional reduction procedure with respect to quality of approximation depends among others just on assumed form of the skeletal dynamical system. We can postulate its form arbitrarily admitting possible inconsistencies in approximation of EDS . We can proceed in a more advanced form taking into account discussed above premisses. There is imaginable also a mathematical derivation of the form of SDS following from mathematical structure of the elementary dynamical system.

Let us discuss a concept of identification of constants which are present in $SDS(\mathbf{C})$ in order to obtain RDS . Let $C = \{\psi(t) : \psi \in \bar{\mathcal{M}}, t \in T\}$ be a space of continuous time processes in $\bar{\mathcal{M}}$ with a metric $\rho : C \times C \rightarrow R_+ \cup \{0\}$. We can construct two kinds of processes. The first one is based on solution $\varphi(\varphi_0, \mathbf{f})(t)$ of equation (19) and has the form $\pi_T(\varphi(\varphi_0, \mathbf{f})(t))$. The second one is created by the skeletal dynamical system with assumed constants \mathbf{C} . Thus, we have a solution of equations of SDS as $\mathbf{d}(\mathbf{C}, \pi(\varphi_0), \bar{\mathbf{f}})(t)$, where $\bar{\mathbf{f}}(t) = \pi_{fT}(\mathbf{f}(t))$. Let us consider the function

$$h(\varphi_0, \mathbf{f}) = \inf_{\mathbf{C} \in \mathcal{C}_E} \rho(\mathbf{d}(\mathbf{C}, \pi(\varphi_0), \bar{\mathbf{f}})(t), \pi_T(\varphi(\varphi_0, \mathbf{f})(t))), \quad (32)$$

where \mathcal{C}_E is an admissible set of constants.

Let \mathbf{C}^* stands for constants for which the function h attains a minimum. Then, a satisfactory approximation should have the property that \mathbf{C}^* exhibits a weak dependence on φ_0 and \mathbf{f} . This, in turn, is connected with assumed form of functions π_T and SDS which reflects the correctness of averaged modelling. Taking into account the discussed above degree of freedom in approximation we

can obtain a set of \mathbf{C}^* . Finally, we have to choose a constant $\bar{\mathbf{C}}$ from the set of \mathbf{C}^* by an averaging method. Then,

$$\bar{\mathbf{C}} = Av\{\mathbf{C}^*\} \quad (33)$$

where Av means the averaging operation. Obtained constants $\bar{\mathbf{C}}$ determine a dimensionally reduced dynamical system $RDS(\bar{\mathbf{C}})$. By means of Eqs. (32), (33) an approximation and identification procedure denoted further in general as app is established.

We can discuss also another kind of approximation procedure. Let us assume that there is a relation \mathcal{R}_{app} between variables and forces of SDS and constants \mathbf{c}_{EDS} considered in the elementary dynamical system. Let us consider a system of equations

$$\{\bar{\mathcal{L}}_{TG}, \bar{T}_C\}(\mathbf{C}, \mathbf{d}_g, \mathbf{d}_c) = \{\bar{\mathbf{f}}, \mathcal{B}\}, \quad (34)$$

$$\mathcal{R}_{app}(\mathbf{d}_g, \mathbf{d}_c, \bar{\mathbf{f}}, \mathcal{B}_c, \mathbf{c}_{EDS}) = 0. \quad (35)$$

We assume that the equation (34) and the relation \mathcal{R}_{app} create together such a system of equations which enables us to determine $\bar{\mathbf{C}} = \mathbf{C}(\mathbf{c}_{EDS})$. In such a case the reduced dynamical system is also determined. This kind of determination of constants is closer to this one applied in micromechanics for instance [40].

Summing up these considerations let us notice that the following general procedure is established

$$\{EDS, DR\} \rightarrow RDS(\bar{\mathbf{C}}). \quad (36)$$

It means that the dimensional reduction procedure

$$DR = \{\pi_T, \pi_{fT}, SDS, app\} \quad (37)$$

acting on elementary dynamical system (19) leads to obtaining the reduced dynamical system RDS . Consequently, RDS is considered as describing approximately, evolution of our initially introduced physical system.

We tend towards creating the situation when widely applied continuum mechanics approach to modelling various physical systems could cooperate with discrete methods. We would like to have at our disposal also the possibility when various scale continuum models could cooperate within the multiscale system. Thereby, we should show how continuum mechanics emerges from collection of dynamical system approach. Formalization of scale of averaging is also important in this case.

6.3 Remarks on placement of continuum mechanics within collection of dynamical systems

Continuum mechanics is widely applied in mechanics of materials. Such a theory is applied even for very small scale models. Let us mention here the nanoscale

models of plasticity [7] or martensitic transformation [24]. However, with decreasing of scale many effects which are usually discontinuous are revealed. Then, we introduce within the continuum mechanics various additional notions for taking them into account. Let us mention the discontinuity surface considered in a small scale model as slip plane or various kinds of interfaces for phase transition models. Additionally, some effects related to smaller scale can be averaged and then represented by various internal state variables [9,14] in a larger scale. Let us mention here such phenomena as small defects, cracks or dislocations.

Nanoscale continuum models are rather complex in comparison with larger scale continuum models. This is manifested by the presence of larger number of constants which should be determined in order to determine entirely the model with a smaller scale. On the other hand it is difficult to carry out experiments related precisely to separate small scale phenomena in materials in order to determine mentioned constants. Therefore, a possible way for identification of constants is cooperation of molecular dynamics and nanoscale models within a two-scale model just in order to solve this problem.

The last demand needs adjustment of formulation of continuum mechanics for realization of the dimensional reduction procedure. Let us note that fields on continuum create infinite-dimensional spaces. On the other hand, models of molecular dynamics are finite dimensional. This is formal difficulty in viewing continuum models which are physically simpler, as more averaged and obtained by means of the dimensional reduction procedure from the molecular dynamics. Therefore, classical formulation of axioms of continuum mechanics should be modified into the case when fields on continuum would be finite dimensional.

Method of introducing finite dimensional fields consists in assumption on validity of balance equations not for all subbodies of the body \mathcal{B} as in classical formulation of continuum mechanics [39], but only for their determined finite family \mathcal{K} . It is in fact a generalization of the classical formulation since all subbodies create a particular case of \mathcal{K} .

We try to introduce continuum in relation to an elementary dynamical system (18). In order to do it we introduce the mapping G_K associated with the division of EDS into collection of dynamical systems. Consequently, the mapping G_K introduces three-dimensional disjoint subsets of the Euclidean space E_e which will be further interpreted as partition of the body \mathcal{B} to the set of subbodies K_h and $\bigcup K_h$. Thereby $G_K(\{\varphi_h\}(t)) = \{K_h\}(t)$ describes evolution of $\mathcal{B}(t) = \bigcup_h K_h(t)$ in time. $K_h(t)$ will be also denoted by $\chi_t(K_h)$ in what follows.

Definition 6.1 The body associated with the dynamical system $\dot{\varphi} = L(\varphi, \mathbf{f})$ is defined with the help of mapping G_K as $\mathcal{B}_\varphi = \bigcup_{h \in I_P} K_h$.

Let $\bar{V}_D = \{\{\bar{\chi}, a\} : \{\bar{\chi}, a\} = \{\chi_h, a_h\}, h \in I_P\}$, where a_h is a function determined on the set $\{\chi_j\}$ and designed to take into account relations of value of the deformation function assigned to h -th subsystem with other neighboring subsystems.

Let us define the space V_κ of deformation functions χ_κ of the body \mathcal{B} with respect to a given configuration κ as $V_\kappa = \{\chi_\kappa : \chi_\kappa = \lambda \circ \kappa^{-1}, \lambda, \kappa \in \mathcal{C}\}$, where \mathcal{C} is the placement of the body in Euclidean space E_e in a similar way as this is done in classical formulation of continuum mechanics [14,39,41]. Let furthermore, $\alpha_\chi : \bar{V}_D \rightarrow V_\kappa$ be a function and $\chi_\kappa^\mathcal{K} = \alpha_\chi(\{\chi_h, a_h\})$, $\chi_\kappa^\mathcal{K}(\mathbf{X}_h) = \chi_h$.

Definition 6.2 The deformation function associated with the distinguished family of subbodies \mathcal{K} is a function $\chi_\kappa^\mathcal{K}$ of the form $\chi_\kappa^\mathcal{K} = \alpha_\chi(\{\chi_h, a_h\})$.

Definition 6.3 The motion of the body \mathcal{B} associated with the family of sets \mathcal{K} is a continuous map $\chi_t : [0, T] \rightarrow \{\chi_\kappa^\mathcal{K}\}$.

With the help of above definitions we have obtained deformation function and motion of the body in connection with the elementary dynamical system. We also introduce a function \bar{T} on \mathcal{K} , which represents temperature, as $\bar{T} : \mathcal{K} \rightarrow R^P$, $\bar{T}(\{K_h\}) = \{T_h\}$. However, temperature has not as clear geometrical interpretation as the deformation function. We have discussed relation of the deformation function to the elementary dynamical system. Therefore, we should also discuss concisely the relation of temperature to elementary dynamical system within this approach. Considerable number of physical systems can be characterized by variables of two types. The first one is related to slowly varying and the second one to quickly varying processes. The most known example is a system with deformation and atomic oscillations represented in an averaged way by temperature.

Motivated by this let us introduce a special case of mapping $\pi_T = \{\pi_{ST}, \pi_{QT}\}$ in which two parts related to slowly and quickly varying variables are discriminated. As a result $\mathbf{d}(t) = \pi_T(\varphi(t))$ can be expressed as $\mathbf{d} = \{\mathbf{d}_S, \mathbf{d}_Q\} = \{\pi_{ST}(\varphi), \pi_{QT}(\varphi)\}$.

Let us assume also that in this discussion, the elementary dynamical system is a Hamiltonian dynamical system (*HDS*) and takes the form

$$\begin{aligned} \frac{d\mathbf{q}_i}{dt} &= \mathbf{v}_i \\ m_i \frac{d\mathbf{v}_i}{dt} &= -\frac{\partial H}{\partial \mathbf{q}_i} + \mathbf{f}_i, \end{aligned} \quad (38)$$

where $i \in I_N = \{1, 2, \dots, N\}$, H is a Hamiltonian and \mathbf{f}_i is a force acting on i -th material point. Let $\mathbf{q} = \{\mathbf{q}_i\}$, $\mathbf{v} = \{\mathbf{v}_i\}$.

Let us take a set of time instants $t_0 < t_1 < \dots < t_K$ which belong to the time interval $T = [t_0, t_0 + T]$, $t_K = t_0 + T$, and let $I_K = \{0, 1, \dots, K\}$. By means of these instants we divide the time interval into the sum $T = \bigcup_k T_k$, $T_k = [t_{k-1}, t_k]$, $k = 1, \dots, K$. Then, for each k we can calculate the value of $\tilde{\mathbf{q}}_k$ as

$$\tilde{\mathbf{q}}_k = \frac{1}{T_k} \int_{T_k} \mathbf{q}(t) dt . \quad (39)$$

A value $\tilde{\mathbf{q}}_0 = \mathbf{q}(t_0)$ is assigned to $k = 0$. With the aid of the sequence of values $\{\tilde{\mathbf{q}}_k\}$, $k \in I_K$ we can generate a function $\tilde{\mathbf{q}}(t) = I_q(\{\tilde{\mathbf{q}}_k\})$, where I_q is an approximation procedure. Now, we are able to decompose the variable $\mathbf{q}(t)$ into two summands

$$\mathbf{q}(t) = \tilde{\mathbf{q}}(t) + \delta\mathbf{q}(t) . \quad (40)$$

Thus, $\tilde{\mathbf{q}}(t)$ represents the slowly varying part of $\mathbf{q}(t)$ and $\delta\mathbf{q}(t)$ its rapidly varying part.

The question arises what properties should the approximation procedure I_q has in order to describe real slowly varying process in accordance with the introduced set $\{\mathbf{q}_k\}$. Slowly varying variable should gradually change its values between given points. This fact should be expressed by possible small values of the second time derivatives. Consequently, the approximation procedure I_q could be defined as a process of finding a function $\tilde{\mathbf{q}}(t)$ which satisfy the following set of properties:

$$\left\{ \begin{array}{l} I_q(\{\tilde{\mathbf{q}}_k\}) = \tilde{\mathbf{q}}(t) , \\ \sup_{t \in T} (|\frac{\partial^2 \tilde{\mathbf{q}}}{\partial t^2}|) \rightarrow \text{inf} \\ \tilde{\mathbf{q}}(\tau_k) = \tilde{\mathbf{q}}_k , \quad \tau_k = 0.5(t_{k-1} + t_k) , \\ \tilde{\mathbf{q}}(t) \in C^n , \quad n \geq 2 , \quad t \in T . \end{array} \right. \quad (41)$$

It should be expected also that $\int_{T_k} (\mathbf{q} - \tilde{\mathbf{q}}) dt = \int_{T_k} \delta\mathbf{q} dt \approx 0$, where " \approx " means equality with an admissible error. An example of realization of above procedure is given in the paper [42].

We assume here that temperature should be defined within deterministic dynamical system by means of an averaging procedure related to quickly varying displacements of particles expressed at atomistic level. The precise definition of this averaging is not simple since temperature has physical interpretation. Thereby, the definition of temperature should lead to accordance with all effects which are measurable as physical effects related to temperature. Nevertheless, we can discuss formally the field of temperature having in mind above interpretation as related to quickly varying processes.

Let $\bar{V}_{TM} = \{\{\bar{T}, b\} : \{\bar{T}, b\} = \{T_h, b_h\}, h \in I_P\}$, $V_{TM} = \{T(\mathbf{x}) : \mathbf{x} \in \chi(\mathcal{B})\}$, where b_h is function defined on the set $\{T_j\}$ which allow us to take into account

effects of values of T_j from neighboring dynamical system on value of T_h . Role of this function is similar as a_h . Let us consider a function $\alpha_T : \bar{V}_{TM} \rightarrow V_{TM}$ and $T^\mathcal{K} = \alpha_T(\{T_h, b_h\})$.

Definition 6.4 The temperature field $T^\mathcal{K}$ associated with the distinguished family of subbodies \mathcal{K} is the field obtained with the help of the function α_T as $T^\mathcal{K} = \alpha_T(\{T_h, b_h\})$.

The function b_h is important since it enables us to take into account gradients of temperature for instance. This can improve approximation of continuum distribution of temperature by means of the mapping α_T . The function α_χ assigns a deformation function field $\chi_\kappa^\mathcal{K}$ to the set of its discrete values. The aim of this function is to introduce a continuous field χ on the body \mathcal{B} . Similar role plays the function α_T for T . Thus, the spaces of such fields $Im\alpha_\chi \subset V_\kappa$ and $Im\alpha_T \subset V_{TM}$ are finite-dimensional, where $Im\phi$ means the image of the function ϕ .

Our previous discussion on collection of dynamical systems follows existence of a set of notions introduced formally on *EDS*. We admit the existence of functions \tilde{m} , $J_{\varphi ij}$, c_φ , E_φ , $W_{\varphi ij}$, R_φ which introduce masses m_i , efflux of mass J_{ij} , source of mass c_i , efflux of energy W_{ij} and source of energy R_i accompanied by subsystems. Consequently, mentioned functions indexed here by φ are referred directly to the elementary dynamical system. We use these functions to reformulation of general form of balance of mass and energy equations defined for collection of dynamical system to the case of continuum.

Let $\tilde{m} : \mathcal{M}_\Pi \rightarrow \{\{m_h\}\}$ be mapping which determines a set of masses related to collection of dynamical systems. Let $\mathcal{M}_M = \{\{M_h\}\}$ and $M : \mathcal{M}_K \rightarrow \mathcal{M}_M$ be a function which determines masses assigned to K_h . We have also that $\pi_h \circ M(\mathcal{K}) = M_h$, where M_h is the total mass related to K_h . M_h are defined by means of the relation $M \circ G_K = i \circ \tilde{m}$, where i is the identity mapping. Consequently, a system of mass related to continuum is introduced by means of mapping \tilde{m} defined on elementary dynamical system. Let $\mathcal{B} = \bigcup_h K_h$, $h \in I_B$, where $I_B \subset I_P$ is a set of indexes defining an arbitrary subbody \mathcal{B} of the body also denoted by \mathcal{B} . Then, $M(\mathcal{B}) = \sum_{h \in I_B} M_h$. Using this definition we obtain mass related to subbodies as a kind of measure defined on the body.

Energy accompanied by the elementary dynamical system is introduced by means of the function $E_\varphi : \mathcal{M}_\Pi \rightarrow R^P$. Then, energy $\mathcal{E} : \mathcal{M}_K \rightarrow \{\mathcal{E}_h\}$, $\mathcal{E}_h = \pi_h \circ \mathcal{E}(\{K_h\})$ assigned to each K_h , is defined by means of the relation $\mathcal{E} \circ G_K = i \circ E_\varphi$. As a result, we are able to define energy related to subbody as $\mathcal{E}(\mathcal{B}) = \sum_h \mathcal{E}_h$. We assume further that $\mathcal{E} = E + \mathcal{T}$ is a sum of internal energy and kinetic energy. Source of mass $c_\varphi : \mathcal{M}_\Pi \rightarrow R^P$ and source of energy $R_\varphi : \mathcal{M}_\Pi \rightarrow R^P$ are defined now as $C : \mathcal{M}_K \rightarrow R^P$, $R : \mathcal{M}_K \rightarrow R^P$ by

means of relations $C \circ G_K = i \circ c_\varphi$ and $R \circ G_K = i \circ R_\varphi$. These quantities are defined for subbodies by means of expressions $C(\mathcal{B}) = \sum_h C_h$, $R(\mathcal{B}) = \sum_h R_h$. Efflux of mass $J_{\varphi ij} : \mathcal{M}_\Pi \rightarrow R$ and efflux of energy $W_{\varphi ij} : \mathcal{M}_\Pi \rightarrow R$ are defined as $J_{ij} : K_i \times K_j \rightarrow R$, where J_{ij} is determined by means of $J_{ij} \circ (G_{K_i} \times G_{K_j}) = i \circ J_{\varphi ij}$ and $W_{ij} : K_i \times K_j \rightarrow R$, where we obtain W_{ij} from $W_{ij} \circ (G_{K_i} \times G_{K_j}) = i \circ W_{\varphi ij}$.

Let us consider the boundary of the body $\partial\mathcal{B} = \partial \bigcup_h K_h$. Then, $J(\partial\mathcal{B}) = \sum_{i \in I_B, m \in I_P - I_B} J_{im}$ and $W(\partial\mathcal{B}) = \sum_{i \in I_B, m \in I_P - I_B} W_{im}$.

We consider also $\partial\mathcal{B}_s \subset \partial\mathcal{B}$ which is defined as $\partial\mathcal{B}_s = \bigcup_{h \in I_s} (\partial K_h \cap \partial\mathcal{B})$, $I_s \subset I_B$. There exists relation between $\partial\mathcal{B}_s$ and a set of J_{im} . We assume that the pair of indexes $\{i, m\}$ is associated with $\partial\mathcal{B}_s$ if $\partial\mathcal{B}_s$ is a border between subsystems i and m . Then, $J(\partial\mathcal{B}_s) = \sum_{i \in I_s, m \in I_{s_i}} J_{im}$. With the help of introduced functions, the balance of mass equation (21) interpreted in terms of continuum is given by

$$\dot{M}(\mathcal{B}) + J(\partial\mathcal{B}) - C(\mathcal{B}) = 0. \quad (42)$$

with the additional condition satisfied for arbitrary $\partial\mathcal{B}_s \subset \partial\mathcal{B}$

$$J(\partial\mathcal{B}_s) = \bar{J}(\partial\mathcal{B}_s). \quad (43)$$

The balance of energy equation (24) expressed in terms of continuum is assumed in the following form

$$\dot{E}(\mathcal{B}) + \dot{T}(\mathcal{B}) + W(\partial\mathcal{B}) - R(\mathcal{B}) = 0, \quad (44)$$

with the additional condition satisfied for arbitrary $\partial\mathcal{B}_s \subset \partial\mathcal{B}$

$$W(\partial\mathcal{B}_s) = \bar{W}(\partial\mathcal{B}_s). \quad (45)$$

Neglecting at the moment detailed representations of introduced below quantities, we formulate also the second law of thermodynamics as a supplementary postulate. This is given with the help of the balance entropy expressed as

$$P(\mathcal{B}) = \dot{S}(\mathcal{B}) + H(\partial\mathcal{B}) - N(\mathcal{B}) \geq 0, \quad (46)$$

where S is entropy, H is efflux of entropy and N stands for the source of entropy. P represents production of this quantity.

Detailed continuum models can be considered when we introduce representations of quantities appearing in balance equations. Let us note that obtained models are considered for chosen family of subbodies \mathcal{K} . This induces that spaces of fields on continuum are finite-dimensional. It means in turn that our continuum models are directly finite-dimensional and no discretization procedure should be applied.

Formulated on this way continuum models can be considered within multi-scale modelling since, owing to their finite-dimensionality, they can be applied as

a result of the dimensional reduction procedure. In particular, they can cooperate with other discrete methods within multiscale approach. Therefore, unified approach of molecular dynamics and continuum mechanics for solids can be discussed [42].

When we apply multiscale modelling with continuum approach on the reduced level then we have to determine skeletal dynamical system. Premises for formulation of this system follow from the aware option of scale of averaging which is expressed by the family of subbodies \mathcal{K} . Let us note that a similarity with discretization method appears here. In both cases we obtain finite-dimensional dynamical systems. We can also choose as \mathcal{K} a family of finite elements which can be interpreted as a set of subbodies. However, in the case considered in this paper we define equations without intermediate stage which is done by an infinite-dimensional continuum dynamical system which needs discretization.

Formally we can also introduce the skeletal dynamical system by a discretization of infinite-dimensional model. Then, scale of averaging will depend on the size of finite elements applied. However, since the scale of averaging was not determined formally for the infinite-dimensional model than we are not sure whether the constitutive equations are correct in relation to the scale of averaging. Form of constitutive equations is just most dependent on the scale of averaging applied.

7 Role of multiscale mechanics of materials for thermal barrier coatings

Thermal barrier coatings can have miscellaneous structures. They can be complex which can be expressed in relation to various scales. Thereby, it justifies modelling of properties and behavior of TBC by means of multiscale mechanics.

Thermal cycles and multilayer structure of thermal barrier coatings produce stresses induced by frequently different thermal expansion of separate layers. Then, ability to stress relaxation has connections with inelastic deformation. Mechanisms of inelastic deformation can be various. We can consider slips at nanoscale level. We can consider slip bands corresponding rather to microscale. Porous structure needs considerations of inelastic deformation in larger scale than the previous ones. Superplasticity should also be taken into account for appropriate range of temperatures. Then dynamical properties of interactions between grains can be discussed also in relation to various scales.

Resistance of TBC against fracture and finally against damage is of key importance. As a result modelling of crack propagation within multilayer structure of TBC at various scales can provide premises for design of TBC. Stress distribution in zone near crack tip can be considered with various degree of approximation. In particular we can have to do with martensitic transformation in this region.

Small grains of partially stabilized zirconia can be transformed into monoclinic phase due to stresses near the crack tip. As a result of this, stresses in the zone decreases and crack propagation is stopped. This leads to increasing of toughness. Thereby, we are able to design tougheness by controlling form and distribution of grains of tetragonal phase dispersed in the cubic one in YPSZ [19].

Thermal properties of TBC are associated with thermal conductance which should be lowered to a possibly small extent. Thus, various types of microstructure or even nanostructure can affect this property. We can decrease directly thermal conductivity of material by modification of microstructure or produce a porous structure which also decreases thermal conductivity.

Larger temperatures at which TBC works need consideration of thermal radiation and ability to reflect this radiation. In such case, especially the multilayer structures can be useful [38]. Let us note that thermal properties should be designed together with mechanical ones since durability of TBC is very important for its practical use.

Above discussion accentuates the role of a variety of phenomena which are important for correct operation of TBC. This discussion indicates also which phenomena should be modelled and which scale should be applied. In particular the martensitic transformation is of great importance especially at nanoscale level. Let us note that nanoscale model of the martensitic transformation has been developed in several papers [9, 24] mainly in case of shape memory alloys based on copper. Therefore, it would be well justified to extend such models to the case of ceramic materials and especially to the case of zirconia and partially stabilized zirconia.

Nanoscale models of slip plasticity have been discussed in [7, 9]. Furthermore, extension of this approach to the case of cooperation of slip plasticity and martensitic transformation at the nanoscale level is done in [9, 25]. Development of such approach could be convenient especially for possible plastic deformation of cubic matrix of zirconia which has considerable component of yttria. Within this phase the tetragonal grains with smaller content of yttria are produced. Then, cooperation of plasticity and martensitic transformation is also imaginable in a similar manner as in [25]. We can suspect also some additional mechanisms of inelastic deformation in zirconia-yttria system. They can be similar to superplasticity or even to be superplasticity for appropriate temperature range. Then, nanoscale modelling seems to be adequate in order to reflect mechanisms of this kind of inelastic deformation.

In so complex environment of phenomena as discussed above we should model the fracture. In order to reflect correctly stresses near the tip of the crack we should have at our disposal models which reflect, with appropriate precision, all effects of inelastic deformation in this zone. This suggests also application

of nanoscale modelling of crack propagation. Such a model has been discussed in [8]. We can introduce nanoscale models phenomenologically by postulating variables and constitutive equations. However, it seems that finally cooperation between molecular dynamics and nanoscale modelling is inevitable. We have to do with considerable temperature changes in case of TBC. This accentuates the role of thermal processes within mechanisms of inelastic deformation. Molecular dynamics is just appropriate for simulation of this kind of phenomena.

Let us note that produced TBC layer is not homogeneous. It has frequently pores or it is a multilayer structure. Then, the nanoscale models of a small part of material which is placed within the layer is responsible for a part of TBC properties. Therefore, we should discuss the problem how composition of various, different smaller parts of TBC creates new more averaged properties. We promote the multiscale approach. Therefore, we should discuss possibility of placement of a nonhomogeneous structure within the collection of dynamical systems. Let us assume that we consider as an elementary dynamical system a nanoscale model. Then, in case of nonhomogeneity of structure only a small part is represented by our nanoscale model. In general, nonhomogeneity means in this case that various nanoscale models can be applied to different parts of material which can next have to be averaged. Let us consider a set of mappings $\pi_{H\alpha}$ representing in our discussion various applied nanoscale models related to homogeneous with respect to modelling parts. Then, the whole mapping π_{NH} corresponding to nonhomogeneous material is expressed by

$$\pi_{NH} = \mathcal{H}(\Pi_{\alpha}\pi_{H\alpha}) , \quad (47)$$

where Π stand for the product of mapping operation. Thereby, skeletal dynamical systems for nonhomogeneous material should be built on basis of possible smaller homogeneous systems taking into account new qualitative effects corresponding to the new scale which is expressed just by mapping \mathcal{H} .

We have discussed a variety of phenomena which we can encounter in thermal barrier coatings during their operation. Furthermore, we have indicated problems associated with modelling of such phenomena. The first conclusion is that we suggest nanoscale methods for modelling considered as a main segment of multiscale approach for description of TBC. Such an approach seems to be the most convenient since mechanisms of inelastic deformation are frequently well expressed just in nanoscale. Let us notice that we cannot or should not apply the full multiscale approach to each designed thermal barrier coating. First, it can be very complex. Furthermore, methods of design can be sometimes restricted to some averaged effects. We should be aware however which scale of averaging is appropriate for our needs in the design.

Full multiscale approach seems to be rather a distant perspective. We have to built first particular nanoscale models for various phenomena. Next, we should

elaborate ways for construction of skeletal dynamical systems for various methods of averaging. Cooperation with molecular dynamics within multiscale approach is viewed also as a large area for investigation.

The next conclusion is associated with nanoscale modelling and their particular role. It would be convenient to have at our disposal entirely developed nanoscale models of materials which could be applied in TBC design and valid for the whole range of phenomena which we can expect during the TBC operation. It accentuates the necessity of independent development of nanoscale modelling for inelastic deformation in metals, alloys and ceramics.

8 Concept of unified description of the deposition process and behavior of thermal barrier coatings

We have discussed above the need for description of behavior of thermal barrier coatings within multiscale method of modelling in mechanics of materials. Having such a description at our disposal we are able to express a design criteria as it was discussed in Section 3.

We try to suggest a way which would be viewed as unified description of production as well as mechanical behavior of thermal barrier coatings. The aim of such a unification is achievement of possibility of design of TBC in order to translate, in the next step, the design criteria into mathematically expressed properties of the deposition process. Then, we would also obtain a criteria for design of the deposition process. All this is aimed at production of thermal barrier coatings with required properties. We assume that two segments of this unification are of key importance. The first one is represented by the possibility of expression of design criteria for TBC. The second one is manifested by notion of index of structure which inform us to what degree the method of production of TBC layers is associated with initial preparation and realization of the deposition process. We should discuss relations between mentioned two segments of mathematical modelling. Let us notice that criteria for design are frequently related to a critical condition for some phenomena. Let us mention here plastic deformation by slip for instance. Initiation of slip is expressed by attaining a critical value of stresses obtained during elastic deformation. Attaining of the critical condition changes quality in behavior of material.

When we design a material we usually would like to obtain the resistance against a process viewed as a property of this material. Critical condition for crack initiation for instance, is also very important design criterion. However, let us notice that discussed above criteria have various forms for various scale models. The question is which criteria should be considered. Let us note that preparation of the deposition process also depends on scale. In this case we have to do with

the scale related to controlling of preparation of structure of material for deposition and with the scale associated with modelling of such process. It seems that scale associated with design criteria should be associated with the scale which is controlled during preparation and deposition process. However, this is not entirely clear. Design of materials is associated with atomic composition and also with larger its structures such as grains of single crystal for instance. Thus, it is inevitable to discuss arrangement of atomic structure even in the case when we are not able to control them precisely. Consequently, the best criteria for material design are related to atomic scale.

Let us note also that controlling of preparation and realization of the deposition process can be associated with varying scale. At first stage we can prepare a powder for instance, having grains of a given size. Next it can be deposited with a determined precision which frequently leads to production of pores. However, post-deposition process can also lead to recrystallization recovering a small scale structure. All this support multiscale modelling of the preparation of deposition, the deposition process as well as multiscale approach to modelling and design of thermal barrier coating including even atomic scale.

Let us note that the free energy is an important mathematical object which is present in models related to various scales. By means of this function we are able to express various critical conditions. Let us mention for instance critical condition for slip activation in a nanoscale model [7]. Within this model even slip systems are defined by means of the free energy.

Tending towards unified multiscale approach to description of miscellaneous phenomena in materials we postulate within nanoscale models critical conditions for initiation of martensitic transformation and initiation of crack propagation also by means of the free energy. Therefore, free energy is viewed as having convenient properties for creating unified theoretical approaches in mechanics of materials. Thereby, at larger scales than nanoscale we should prefer descriptions having free energy as notion of key importance. Let us mention here a model of plasticity which follows from [14] for instance. Consequently, it would be convenient to use the free energy as an element of index of structure in stage of preparation of grains of powder for instance. We can assume that

$$\mathcal{I}_P = \{\Psi_1, \dots, \Psi_N\}, \quad (48)$$

which means that within this stage of preparation of material, its n -th grains have the free energy $\Psi_n, n = 1, \dots, N$. Then, after the deposition the free energy related to an assumed scale related to a small part of material placed between pores, has the form

$$\Psi = \Phi_D(\Psi_1, \dots, \Psi_N), \quad (49)$$

where the function Φ_D represents the method of transformation of small particles into larger one and calculating the free energy for such a structure.

However, at larger scales we have to do also with various defect and pores in particular. Then, still more averaged free energy should depend also on the index of structure related to deposited material expressed previously by \mathcal{I}_M . Thereby, the free energy is not a pure composition of simpler elements but also depends on new variables. We can express this by

$$\Psi = \Phi_{AV}(\Psi_1, \dots, \Psi_N, \mathcal{I}_M). \quad (50)$$

At this moment we do not specify any variables of the free energy. Rather we try to comment where from the free energy follows.

Let us consider a set of variables of the free energy. For description of deformation we can apply the strain deformation tensor \mathbf{e} . In case of nanoscale models variables are simpler but form of the free energy is more complex. Nevertheless, the deformation by slip for instance, has a more clear structure at nanoscale level than at more averaged description, where at the same material point various slip systems can be activated. Therefore, critical conditions for slip for instance are simpler at the nanoscale level. Let \mathcal{S}_{NC} be a hypersurface in space of strain tensors. Let us assume that when deformation attains this surface a slip is activated on a slip system. Thus, the hypersurface \mathcal{S}_{NC} represents just critical conditions for slip activation.

In case of more averaged model the critical condition can also formally have simple form as the hypersurface in space of strain tensors \mathcal{S}_{AvC} . However, then with attaining the critical conditions many additional processes can be associated. This is so since we have to do with larger degree of averaging. The subprocesses can be represented by internal state variables for instance. Then, attaining of the critical condition on the surface \mathcal{S}_{AvC} can be associated with attaining a manifold \mathcal{M}_ξ by a set of internal state variables ξ .

The free energy is part of the skeletal dynamical system in case of multiscale modelling by collection of dynamical systems. Transition between variables of various scales is realized by means of mapping π as it was discussed in Section 6. The skeletal dynamical system can be postulated arbitrarily in more simpler cases. However, it can be also constructed by analysis of the form of *EDS*. Thereby, we can introduce additionally a mapping π_{CRC} which could be precisely defined within whole multiscale modelling process, which transform critical conditions between scales. Thus we have

$$\pi_{CRC}(\mathcal{S}_{NC}) = \{\mathcal{S}_{AvC}, \mathcal{M}_\xi\} \quad (51)$$

for the case discussed above between nanoscale slip plasticity model and a more averaged plasticity model. Let us accentuate that we use the free energy in more averaged description for determining of the critical condition.

Above discussion presents an idea of π_{CRC} mapping which cannot be in general related to the plastic slip. This mapping represents transition between critical conditions between various scales.

Let us consider the situation when our model of the deposition layer is rather averaged. Then, expression of a designed property at this level can be associated with considerations of the set π_{CRC}^{-1} which represents a variety of structures at a lower scale which leads to the averaged critical condition. Consequently, transition between scales, in case of criterion formulated at larger scale, can provide a space for speculation how to manipulate by structures and also by indexes of structures in order to satisfy the criterion.

Let us accentuate the key role of index of structure in unified modelling of behavior and production of TBC. Indeed, we should be aware where from the structure of deposited layer follows. It appears as a result of application of previously prepared components to the deposition. Process of preparation is not always simple and deserves more attention in modelling. Let us mention the situation when powder is produced, especially in case when we would like to control the nanostructure. Too small particles of powder are not useful for spraying. As a result larger particles are produced. However, then they have controlled nanostructure in separated particles. Such a process is called the nanostructurization [43].

Consequently the index of structure

$$\mathcal{I}_{PREP} = \{\mathcal{I}_{P1}, \dots, \mathcal{I}_{Pn}\}, \quad \mathcal{I}_{Pi} = \mathcal{I}_{Nanostr} \quad (52)$$

should have a part $\mathcal{I}_{Nanostr}$ related to nanostructurization. In case when part of $\mathcal{I}_{Nanostr}$ contains also the free energy for such a powder particle then the problem of modelling of preparation of powder particles can be complex.

Further role of index of structure is also important. Especially relation between \mathcal{I}_S and \mathcal{I}_M which are not entirely independent is important. Let us note that mentioned indexes also depend on the scale of averaging applied in modelling of the deposition process. It has been discussed in [6], where evolution of deposited surface is described mathematically.

We can schematically summarize our considerations by introduction of some operations. Let

$$\mathcal{I}_{\alpha+1} = \mathcal{O}_{\alpha}(\mathcal{I}_{\alpha}), \quad (53)$$

where \mathcal{O}_{α} is a mapping transforming index of structure \mathcal{I}_{α} corresponding to a stage α into index of structure $\mathcal{I}_{\alpha+1}$ corresponding to a stage $\alpha + 1$. Then, whole transformation of indexes of structure is expressed by

$$\mathcal{I}_F = \mathcal{O}_{\alpha_F} \circ \dots \circ \mathcal{O}_{\alpha+1} \circ \mathcal{O}_{\alpha} \circ \dots \circ \mathcal{O}_{\alpha_I}(\mathcal{I}_I) = \mathcal{O}_T(\mathcal{I}_I). \quad (54)$$

Then, the mapping \mathcal{O}_T represents transformation of initial index of structure into its final form and represents the whole technological process including deposition.

Unification of theoretical approach would be expressed concisely as finding the relation between π_{CRC}^{-1} and \mathcal{O}_T^{-1} .

Above discussion has been devoted to expression of concept of unified description of the deposition process as well as behavior of the deposited layer. Intention of such unification is to create a theoretical environment for engineering activity related to design of thermal barrier coatings form and its production.

9 Final remarks

Discussion carried out in this paper shows that theoretical modelling of production and behavior of thermal barrier coatings is a complex problem. Controlling of the deposition process is necessary in order to obtain appropriate structures of layers. Furthermore, we should also control what is deposited. Therefore, modelling of preparation of structure of material for deposition also should be theoretically described. Profits from such modelling rest on possibility of expression requirements related to way of preparation of powder for instance, basing on previously determined aims on properties which the TBC layer should have as final product.

Complexity of phenomena in materials creating thermal barrier coatings such as for instance martensitic transformation, inelastic deformation based on various mechanisms, possible superplasticity, considerable role of temperature in all mentioned processes indicate that nanoscale mechanics of materials should be applied.

Application of nanoscale in modelling allows us to model exactly particular mechanisms responsible for mentioned above phenomena. Construction of nanoscale models can be carried out phenomenologically. Then, nanoscale models can be produced for needs directly following from particular phenomena. More advanced approach which is also much more complex consists in application of two-scale method of modelling which contains nanoscale model as a skeletal dynamical system and molecular dynamics method placed in elementary dynamical system. It is expected that such an approach would be useful for explanation of more complex phenomena in relation to temperature. Above discussion indicates that thermal barrier coatings provides reasons for development of nanoscale mechanics of materials and multiscale approach.

This paper shows possible way which would theoretically unify the process of design and production of thermal barrier coatings. This approach, in a sufficiently advanced stage of development, would create theoretical environment for discussion of premises on improvements of the deposition process and the whole production of thermal barrier coatings.

Summarizing, we try to accentuate the fact that the aim of this paper is not devoted to solve problems of a particular thermal barrier coating. In my opinion we have to do with a more general question how to transfer engineering activity

to objects smaller than those considered usually by engineers. Let us notice also that nowadays nanotechnology develops as promising direction just in relation to smaller objects. However, the question how to support nanotechnology by theoretical investigations is rather open. Frequently, traditional methods of mechanics are applied. The question of more precise formalization of theoretical description in this direction is rather not discussed. Let us mention for instance that scale of averaging is not usually discussed when equations are applied. Therefore, promoting thermal barrier coatings we have also opportunity to consider problems of modelling viewed as a base for design at various scales. This paper accentuates necessity of development of methods of modelling by formalization of scale of averaging among others. This paper presents also the point of view of the author on the context of modelling which thermal barrier coatings should have.

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