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# On the Significance of Structure-Property Relationships

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**Abstract.** The importance of deep knowledge of structural information in materials engineering is explained and discussed. Some basic relations, like Hall-Petch relation or linear dependency of hardness and phase composition are presented and discussed. Simultaneously, the difficulties in precise development of structure-property relationships are explained and selected examples of works devoted to structure-property relationships are discussed.

## Introduction

If we analyze either the lectures or textbooks devoted to materials engineering, we always hear or read two terms: properties and structure. This is typical for old as well as for modern lectures and textbooks [1-3]. In commercial applications extremely important is also a price or production cost, but this item is not discussed in this paper. Properties describe and usually quantify the behavior of the materials under various loads and in various environments. So, properties constitute possibly the most important set of information for the potential user of the material. Usually, properties are discussed in conjunction with technological operations that allow for obtainment or modification of them.

The students are also forced to learn about the microstructure. Unfortunately, in most cases they have a lot of difficulty to answer a very simple question: Why microstructure is so important for the material? A typical answer is that microstructure decides what are the properties, but without any deeper analysis or understanding. Surprisingly, this is almost impossible to find clear and straightforward explanation of the importance of our knowledge about materials structure. Although this is not expressed in formal way, materials engineering is based on a fundamental theorem:

*Two materials of identical (micro)structure have identical properties, irrespective of their origin and technological history.*

The above presented theorem has no formal proof, but it is a quintessence of thousands years of experimental observations. A natural consequence of this theorem is looking for precise structure-property relationships. Having such relations coupled with the knowledge how technological processes modify (micro)structure, one can precisely choose technological operations leading to anticipated properties.

## Selected basic structure-property relationships

A good example of structure-property relationship that has both theoretical background and satisfactory experimental verification is analysis of tensile strength of a dual-phase material (Fig. 1). We have two phases: phase A of high strength and phase B of low strength. The simplest case is a material with phases distributed in series. In this case the maximum possible tensile strength is equal to the strength of a weaker phase. It can be even lower if only the phase interface is very weak. Many layered materials used in civil engineering (for example, insulating foam covered by thin metallic or polymer sheets) can be good specimens. In these materials their strength in direction perpendicular to the external surface is very weak.

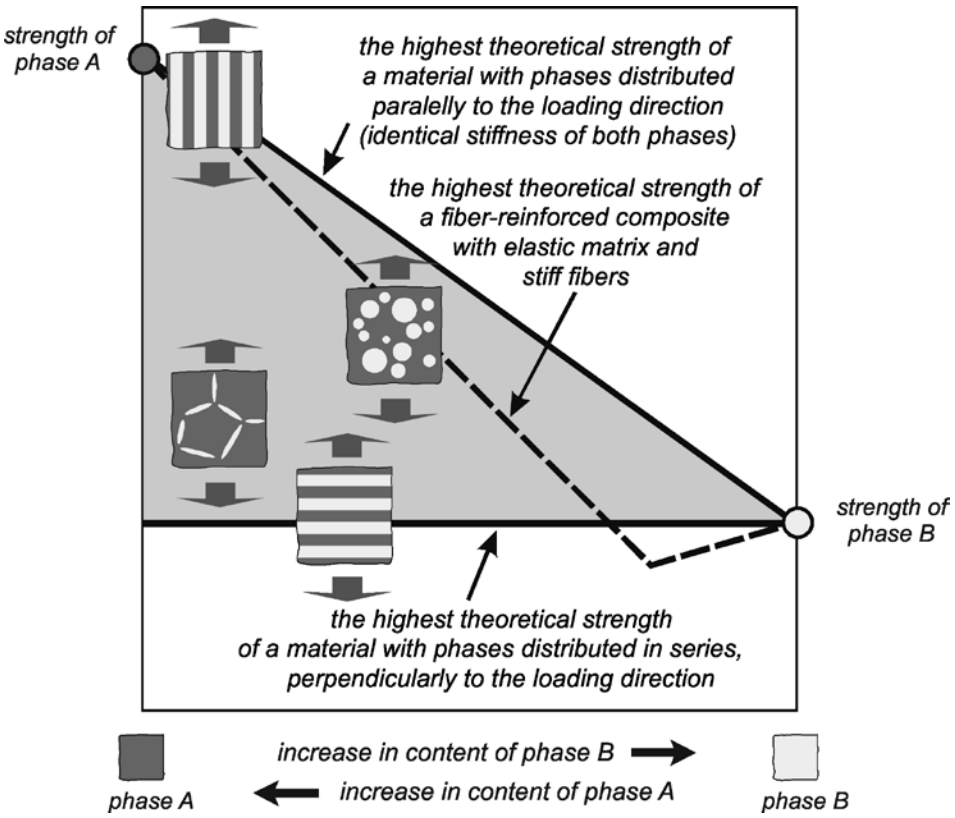


*Fig. 1. Tensile strength of dual-phase materials. Details in the text.*

Another extreme case is tensile strength of a material with phases distributed parallel to the loading direction (Fig. 1). If only the Young modulus is approximately equal in both phases, the final strength is equal to the weighted mean of values for both phases:

$$\sigma_T = V_V(A) * \sigma_T(A) + V_V(B) * \sigma_T(B) \quad (1)$$

where the symbols denote: tensile strength of the material, fraction of phase A, strength of phase A, fraction of phase B and strength of phase B, respectively.

The conclusion is that the material that is built of two phases has never strength higher than strength of these phases. However, this can be a good solution if one phase is resistant and very brittle and the second one has low strength but good plastic properties. Such a combination one can meet in pearlite in carbon steels (lamellar structure that consists of brittle cementite $Fe_3C$ and ductile, soft ferrite) and many fiber-reinforced composites, for example glass fiber with polyester matrix. Unfortunately, in this case we have significant difference in the stiffness of both components (fiber are more stiff). In such a case practically all the loads are transmitted by fibers. On the other hand, in the case of very small amount of fibers they will be broken first and this leads to weakening the of matrix. In some cases a fiber-reinforced composite can be even less strong than the matrix (see dashed line in Fig. 1).

In the case of brittle fibers they have to be fully surrounded by a ductile matrix and therefore the optimum content of fibers is limited. In real composites the effect of fiber contents on the tensile strength is different than this one presented in simplified model (Fig.1). However, one can observe a

local minimum in strength [3]. To conclude, even the simplified model presented above predicts the existence of optimum fiber content in fiber-reinforced composites.

One can meet also dual-phase structures with more complex arrangement of constituent phases. Considering one of them as a matrix, the second one can be distributed in a form of separated particles of different shape or in a form of more or less continuous network. The properties of such materials can be significantly different. A classic example is grey cast iron. Nodular graphite assures tensile strength comparable with steels, whereas flake graphite results in tensile strength 2-3 times lower.

Good agreement with the simple model presented in Fig. 1 demonstrates also carbon steel (part of the Fe-C equilibrium system with carbon contents up to approximately 1.2 %). In the case of ferrite-pearlite structure the tensile strength is proportional to the contents of pearlite, reaching maximum for pure pearlite (0.77 %C). Above this contents of carbon a network of brittle secondary cementite ($Fe_3C$) causes embrittlement of the whole material.

This is also noteworthy, that relation analogous to equation (1) describes well hardness of dual-phase materials. In the case of hardness, it can be also adapted for multiphase materials.

Another well documented relation bounds grain size and yield point. Hall [4] noticed that grain size establishes limit for slip space for dislocations responsible for plastic deformation of mild steels. Independently, Petch [5] obtained a similar relation, but his work concentrated more on brittle fracture. Their results are fully consistent and therefore this important relationship is named after both, Hall and Petch. The Hall-Petch relation illustrates experimental observation that yield point increases with decreasing grain size and can be expressed as:

$$\sigma = a + b * \sqrt{S_V} \tag{2}$$

where: $\sigma$ - yield point of the material, a and b – constant values that depend on the material, $S_V$ – specific surface of grain boundaries (ratio between surface area of grain boundaries and volume of the material).

The Hall-Petch relation also has limitations. In the case of extremely small grains (nan grains), smaller than approximately 1 micrometer, the yield point either remains constant or decreases with the decreasing grain size. So, this is opposite tendency if compared with equation (2) and therefore is called reverse Hall-Petch relation.

The above presented analysis demonstrates that even the simplest structure-property relations can highly non-linear and difficult to establish.

## Stereology as a tool for microstructure quantification

In order to build analytical structure-property relations one need to quantify microstructure. In other words, we necessitate objective measures that allow to characterize microstructure by numbers. Appropriate solutions are given by stereology that defines both appropriate measures and tools for their evaluation. The principles of stereology are well described in the world famous monograph by Ervin E. Underwood [6]. In spite of big progress in measurement techniques only few procedures for microstructure quantification have been standardized. In metallography one can find ASTM standards for evaluation of grain size, non-metallic inclusions in steels or graphite in cast iron. The measurements are used mainly for quality control. Taking into account the theorem presented in *Introduction* to this paper this is postulated that materials showing similar results in quantitative microstructure control have also similar properties. This is noteworthy that from such quality control there is a long distance to development of structure-property relationship. Currently, quantification of microstructures is often automated thanks to image analysis equipment and software. In dedicated software appropriate procedures for typical structures and standardized methods are pre-defined and

ready to use. However, in many cases one have to develop own procedures. Numerous solutions, described and explained step-by-step can be found in the monograph [7].

Development of structure-property relations on the basis of theoretical consideration is very difficult, as our analytical models are usually too simplified. Successful solutions are usually limited to a narrow group of materials, however differences between theoretical and real results can be surprisingly small. More common is the use of statistical analysis for establishing correlations between structural parameters and properties. One example can be evaluation of the effect of trabecular bone on compression strength of vertebral bodies in spine. On the basis of quantitative data from 3D micro tomography [8] the following relation can be evaluated:

$$R_T = 93.308\, V_V - 0.771\, N_V + 22.438\, degr - 2.77 \quad (3)$$

where: $R_T$ – compression strength [MPa], $V_V$ – volume fraction of bone branches, $N_V$ – relative number of junction points [1/mm$^3$] and *degr* – degradation coefficient; ratio between end points and junction points of bone branches.

The above presented equation gives very good correlation between the apparent and evaluated values with correlation coefficient r = 0.952 and mean relative error γ = 0.0952. Stereological parameters are used in this equation. However, it is difficult for physical interpretation, what is a weakness of statistical analysis. Nevertheless, closer analysis of this equation allows for postulating that the volume of bone branches is responsible for nearly 80 % of the bone strength.

## Other examples

Shen and co-authors [9] demonstrated that the properties of the nanocomposites are determined by the intrinsic structure. The experimental results showed that the attapulgite silicates caused that the polymer network exhibits reinforcement in thermal and mechanical properties and slower relaxation in segments mobility compared with neat polyamides. The authors present many results of a wide spectrum of experiments. However, no clear structure-property relation has been established.

Ivanciuc and co-authors [10] presented a sophisticated method starting from molecular level analysis and obtained satisfactory approximation of numerous parameters, like, for example: boiling temperature, molar heat capacity, standard Gibbs energy, density and other quantities for alkanes. Their work was based on numerous computer programs used in chemistry.

Cheng and Ma [11] presented an extended work on properties of metallic glasses. They concluded that in these materials it is extremely difficult to investigate structure-property relationships as they have amorphous structure. Analysis of structure-property relationships is based on local non-homogeneity in distribution of single atoms and local structural organization. Some systematic relations were discovered, however they had rather qualitative character. This work demonstrated how both difficult and important analysis of the structure-property dependency is.

Ray and co-authors [12] studied rheological properties of organically modified layered silicate nanocomposites that are strongly influenced by their nanostructure and interfacial characteristics. The nanostructure was investigated by means of transmission electron microscopy and wide-angle X-ray diffraction. The images obtained using electron microscopy demonstrated how difficult such a structure is for any interpretation. Finally, after numerous experiments the authors demonstrated significant differences between two different biodegradable composites. This work also demonstrated that the internal structure of a material is decisive for its properties but precise quantitative characterisation of this effect is very difficult and requires extended further research. Deeper understanding of the structure-property relationship is in this case

necessary for effective design of new nanocomposites or improvement in the already existing ones.

Gangopadhyay and co-authors [13] measured tribological properties of TiN-$MoS_x$ composite coatings and various parameters related to the coating structure. Increase in $MoS_x$ content was associated with decrease in grain size. From the structure-properties relationships viewpoint it was shown that the (Mo+S) content affects Vickers microhardness, critical load during scratch test and wear coefficient. However, each of these relations exhibited different character. Microhardness decreased with growing (Mo+S) content, critical load had a maximum corresponding to higher (Mo+S) values and wear coefficient had a minimum at lower (Mo+S) content. So, only one of these relations was monotonic.

This brief overview demonstrates that structure-property relationships are of interest for various groups of researchers, working on different materials and in different scale – from macro up to nanoscale. In all the cases deep understanding of the material structure is necessary and the structure-property relations has to be individually fitted to the discussed case.

## Conclusions

Structure-property relationships are important for analysis of the properties and development of new or optimized materials of different character. A very complex nature of various processes and relations within materials causes that evaluation of analytical structure-property relations is very difficult. Usually these relations are nonlinear and often even discontinuous. Statistical analysis of the results can give correlation equations that can good results of prediction but simultaneously are almost useless for physical interpretation of the materials behavior. Numerous papers devoted to structure-property relations prove the importance of this problem. However, in most cases no clear analytical relation between structure and properties is possible to be evaluated and presented.

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