0.1 Statistical Deconvolution

For heterogeneous materials, individual phase properties can be determined by the statistical deconvolution applied to histograms of any mechanical property like E modulus, for example. The deconvolution procedure here was adopted from [1] but different minimizing criteria and a different generation of random sets of probability functions were used as will be demonstrated in the following.

Experimental histograms are constructed from all measurements whose number is N^{exp}, using equally spaced N^{bins} bins of the size b (see Fig. 1). Each bin is assigned with a frequency of occurrence f_i^{exp} that can be normalized with respect to the overall number of measurements as f_i^{exp}/N^{exp}. From that, we can compute the experimental probability density function (PDF) as a set of discrete values:

$$P_i^{exp} = \frac{f_i^{exp}}{N^{exp}} \cdot \frac{1}{b}. \tag{1}$$

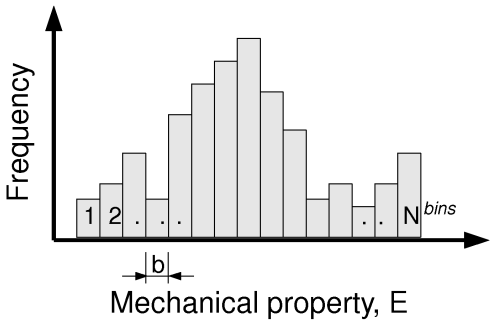

Figure 1: Construction of property histogram with bin size b.

The task of deconvolution into M phases represents finding $j = 1 \dots M$ individual PDFs related to single material phases. If we assume normal (Gauss) distributions, the PDF for a single phase can be written as:

$$p_j(x) = \frac{1}{\sqrt{2\pi s_j^2}} exp \frac{-(x-\mu_j)^2}{2s_j^2} \tag{2}$$

in which μ_j and s_j are the mean value and standard deviation of the j-th phase computed from n_j values as:

$$\mu_j = \frac{1}{n_j} \sum_{k=1}^{n_j} x_k \qquad s_j^2 = \frac{1}{n_j - 1} \sum_{k=1}^{n_j} (x_k - \mu_j)^2 \tag{3}$$

and x is the approximated quantity, i.e. the E modulus in our case. The overall PDF covering all M phases is then:

$$C(x) = \sum_{j=1}^{M} f_j p_j(x) \tag{4}$$

where f_j is the volume fraction of a single phase:

$$f_j = \frac{n_j}{N^{exp}} \tag{5}$$

It was proposed to find individual distributions by minimizing the following error function:

$$min \sum_{i=1}^{N^{bins}} \left[\left(P_i^{exp} - C(x_i) \right) P_i^{exp} \right]^2 \tag{6}$$

in which quadratic deviations between experimental and theoretical PDFs are computed in a set of discrete points that is further weighted by the experimental probability in order to put emphasis on the measurements with a higher occurrence.

For practical computations, the number of mechanically distinct phases M must be known in advance to reduce the computational burden and to give the results a physical meaning. It is usually assessed by some independent measurements, using the knowledge of sample chemistry or simply by detection of several significant peaks in the property histogram. Also the bin size b have to be chosen in advance. Higher value of b leads to more fuzzy histograms with the peaks being smoothed whereas low value of b leads to more precise distributions but the distinctinon between the phases may be harder. In case of structural materials included in this work a reasonable bin size was find to be $b = 1$ GPa and the number of distinct phases M was 1 to 5 depending on a sample.

The minimization in Eq. (6) was based on the random Monte Carlo generation of M probability density functions. They have to satisfy the compatibility condition:

$$\sum_{j=1}^{M} f_j = 1. \tag{7}$$

There is an infinite number of possibilities that can satisfy the condition Eq. (7). So, completely random generation of the sets can lead to a time consuming procedure. In order to guarantee the convergence of the algorithm

and to minimize the computational effort, it is suggessted in this work to use the set of M PDFs in Eq. (2) generated from the experimental dataset of all E moduli. Separation of the dataset into M randomly spaced successive intervals can be done in a straightforward way (see Fig. 2). Mean values, standard deviations in Eq. (3) and volume fractions in Eq. (5) are then computed in these intervals from corresponding E moduli and used in Eq. (4). Then, finding of the set satisfying condition Eq. (6) is a question of a few seconds on a regular PC.

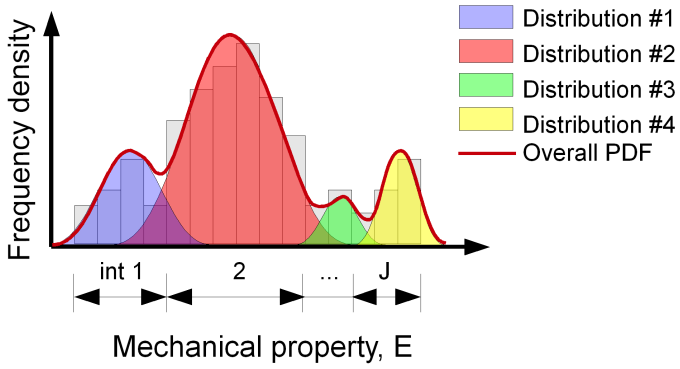

Figure 2: Separation of the experimental dataset to $j = 1 \dots M$ intervals and construction of M probability density functions.

Bibliography

[1] G. Constantinides, K. R. Chandran, F.-J. Ulm, K. V. Vliet, Grid indentation analysis of composite microstructure and mechanics: Principles and validation, Materials Science and Engineering A (430) (2006) 189–202.