Two–colorings of the plane

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1 Introduction

Modern metallic materials frequently consist of crystals of two phases. One of the two phases gives the high strength while the second phase guarantees ductility of the material. Dual-phase materials can be designed for optimum strength-ductility combinations by applying special thermal treatments. Fig.1 shows metallographic sections obtained from microstructures of dual-phase carbon steels after various heat treatments [1]. Inspecting these pictures one can see that all microstructures are made up of structural elements – called grains – of two phases colored white or black. The grains are separated from each other by *grain-boundaries* (i.e. boundaries between grains of the same phase) or *phase boundaries* (i.e. boundaries between grains of different phases). The eight microstructures differ either in the amounts of the white (α-) and the black (β-) phases (the amount of the β-phase increases from the top to the bottom of the two columns) or in the geometrical arrangement of the two phases (the α-grains in the left column (type A microstructures) surround clusters of β-grains which is reversed for the right column (type B microstructures)). By methods originating in stereology such microstructures can be described quantitatively [2]. The parameters obtained by such an analysis are the following :

- volume-fraction; (fraction of area; fraction of length) : $v_V^\alpha, v_V^\beta; (A_A^\alpha, A_A^\beta;\ L_L^\alpha, L_L^\beta)$

$$v_V^\alpha + v_V^\beta = 1 \quad (A_A^\alpha + A_A^\beta = 1;\ L_L^\alpha + L_L^\beta = 1) \tag{1}$$

- mean grain size : $\overline{L}^\alpha$, $\overline{L}^\beta$
- grain contiguity : c^α, c^β [3]
  Contiguity is a measure for the contact of grains of one phase with each other. It is defined as the ratio between the grain boundary area and the total interface area (i.e. grain and phase boundary area) this phase possesses. Contiguity is defined as follows :

$$c^\alpha = \frac{2S_V^{\alpha\alpha}}{2S_V^{\alpha\alpha} + S_V^{\alpha\beta}} = \frac{2P_L^{\alpha\alpha}}{2P_L^{\alpha\alpha} + P_L^{\alpha\beta}}\ ,\quad c^\beta = \frac{2S_V^{\beta\beta}}{2S_V^{\beta\beta} + S_V^{\alpha\beta}} = \frac{2P_L^{\beta\beta}}{2P_L^{\beta\beta} + P_L^{\alpha\beta}}\ , \tag{2}$$

where S_V denotes the respective area per volume of the $\alpha\alpha$- and $\beta\beta$-grain and $\alpha\beta$-phase boundaries. S_V is connected to P_L, the number of intersection points of a straight line with the traces of the boundaries in a plane section, by $S_V = 2P_L$ [3]. In general $c^\alpha + c^\beta \neq 1$.

- mean free path : $\overline{L}^{\alpha\alpha}$, $\overline{L}^{\beta\beta}$
  The mean free path is the average distance between clusters of one phase. It is defined as :

$$\overline{L}^{\alpha\alpha} = \frac{\overline{L}^{\alpha}}{1-c^{\alpha}} \quad , \qquad \overline{L}^{\beta\beta} = \frac{\overline{L}^{\beta}}{1-c^{\beta}} \tag{3}$$

Clearly, for microstructures with $c^\alpha = 0$ or $c^\beta = 0$ (the grains of one phase are completely dispersed in the other phase) the mean free path coincides with the mean grain size.

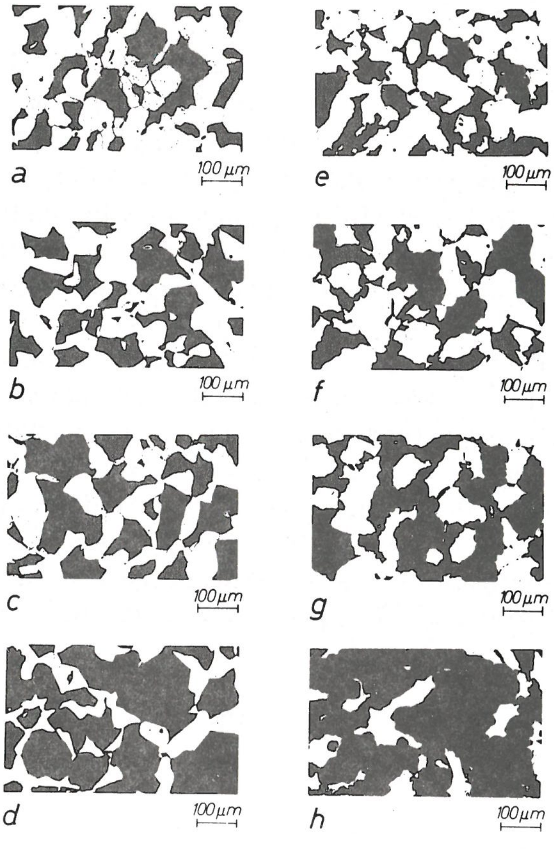

Fig.1 : Microstructure of eight differently heat treated ferritic-martensitic dual-phase steels (after [1]). Left column : type A-, right column : type B-microstructures

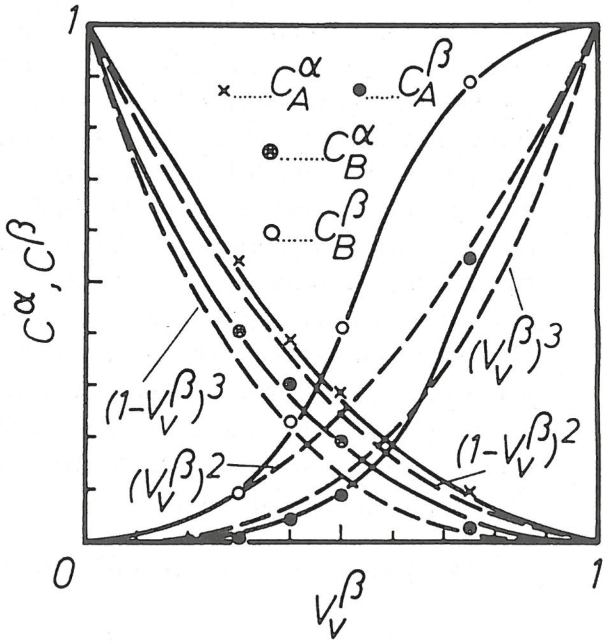

Fig.2 : The stereological parameter contiguity as obtained from the microstructures shown in Fig.1 (after [2]).

Fig.2 shows the results of a quantitative analysis of the microstructures shown in Fig.1 : the parameter contiguity not only depends on the volume fraction of the phases but also on the type of microstructure investigated (A or B) [2]. The concept of grain contiguity has been applied successfully in numerous investigations ranging from electrical resistivity properties to strength and fracture properties of modern engineering materials [4, 5, 6]. The geometrical arrangement of the grains in a two phase mixture is greatly influenced by possible interactions between the grains during thermal treatment of the materials. The strength of the interactions can be quantified by the parameter contiguity as introduced above.

For this reason we seek as the reference solution the random coloring of the plane, i.e. the arrangement of grains of two phases (colors) without interaction between the grains. The grains will be approximated by squares or hexagons.

2 Random two-coloring of the plane

2.1 The linear chain

We consider a linear chain of n α-elements as shown in Fig.3.

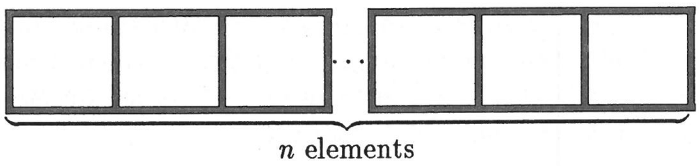

Fig.3 : The linear chain.

k $(1 \leq k \leq n)$ of these elements are randomly painted to become β-elements. Let $A_{k,R}^{1,n}$ denote the number of realizations of each partition $p(k)$ of k containing exactly R components $(1 \leq R \leq k)$. Then

$$A_{k,R}^{1,n} = \binom{k-1}{R-1}\binom{n-k+1}{R} \tag{4}$$

The proof of (4) is as follows. We start with a single block of k β-squares. In order to cut this block into R pieces one has to :
(1) select $R-1$ cutting positions from $k-1$ possible locations in $\binom{k-1}{R-1}$ ways and
(2) place an α-square at the cutting positions.
The remaining $n-k-(R-1)$ α-squares then can be placed in $\binom{n-k-r+1+r+1-1}{n-k-R+1} = \binom{n-k+1}{R}$ ways.

The average number of of β-elements per β-cluster is

$$B^{\beta}(n,k) = \frac{k \cdot \sum\limits_{R=1}^{k} A_{k,R}^{1,n}}{\sum\limits_{R=1}^{k} R \cdot A_{k,R}^{1,n}} = \frac{k\binom{n}{k}}{(n-k+1)\binom{n-1}{k-1}} = \frac{1}{1-\frac{k}{n}+\frac{1}{n}} \tag{5}$$

and for an infinitely long chain :

$$B_{\infty}^{\beta}(L_L^{\beta}) = \lim_{n\to\infty} B^{\beta}(n,k) = \frac{1}{1-L_L^{\beta}} \; . \tag{6}$$

From $\overline{L}^{\beta\beta} = \frac{\overline{L}^{\beta}}{1-c^{\beta}}$ we obtain

$$1 - c^{\beta} = \frac{\overline{L}^{\beta}}{\overline{L}^{\beta} B^{\beta}_{\infty}(k)} , \qquad (7)$$

and thus $c^{\beta} = L^{\beta}_{L}$. Hence random coloring of a linear chain results in a linear dependence of the contiguity on the amount of the considered phase.

2.2 The plane

We consider an $m \times n$ plane of m linear chains of length n containing mn α-elements (squares or hexagons). k $(1 \leq k \leq mn)$ elements are randomly painted to become β-elements. All $\binom{mn}{k}$ realizations are analyzed with respect to $p(k)$ and the number N of β/β-contacts in the β-clusters of each partition $p(k)$. Although the calculations and analyses are done on a high performance double-Transputer computer system the main problems are the CPU-time (several days for a 6×6-field, $1 \leq k \leq 36$) and the bulk of data produced (several megabyte). For these reasons a different approach is followed.

2.2.1 Two linear chains (Square)

We consider two linear chains as shown in Fig.4. There one can see that any two-coloring of the double chain can be interpreted as a word formed from an alphabet of the letters a_{00}, a_{10}, a_{01} and a_{11}.

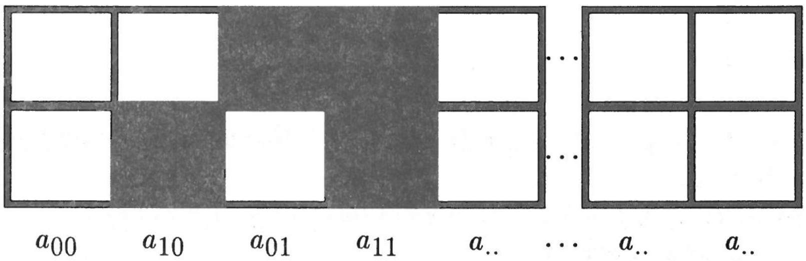

Fig.4 : The double chain. Any coloring can be interpreted as word containing the letters shown above

Thus we try to find solutions to our problem by applying methods from *combinatorics on words* [7, 8].

α) As a special case, we first state the number of words of length n containing only the letters a_{00}, a_{10} and a_{01} and which do not possess the factors $(a_{10}a_{10})$ and $(a_{01}a_{01})$[1]. This number is

$$A^{2,n}_{k,R=k} = 2\sum_{j=0}^{k-1} \binom{k-1}{j}\binom{n-j}{k} , \quad 1 \leq k \leq n \qquad (8)$$

The proof of eqn.(8) was provided by W.Kurth (1989) [9] and is as follows : $2\binom{k-1}{j}$ is the number of words of length k that can be formed from the letters a_{10} and a_{01} containing exactly

[1]This is the total number of realizations possible if k isolated β-squares are placed into the double chain.

j $(1 \leq j \leq k-1)$ factors $(a_{10}a_{10})$ or $(a_{01}a_{01})$. Each of these j illegal factors can be separated by the letter a_{00}. Hence, by doing so the length of the word becomes $k+j$. The $n-k-j$ remaining letters a_{00} can then be placed at $k+1$ positions in $\binom{n-k-j+k+1-1}{n-k-j} = \binom{n-j}{n-k-j} = \binom{n-j}{k}$ ways. Summation over j yields the desired result.

β) Let $A_{k,R}^{2,n}$ denote the number of words of length n that can be formed from r $(0 \leq r \leq \left[\frac{k}{2}\right])$ letters a_{11}, $k-2r$ letters a_{01} or a_{10} and $n-k+r$ letters a_{00}. Furthermore the considered words possess exactly $R-1$ $(1 \leq R \leq k)$ factors $(a_{10}a_{01})$, $(a_{01}a_{10})$, $(a_{11}a_{00})$, $(a_{00}a_{11})$, $(a_{10}a_{00})$, $(a_{00}a_{10})$, $(a_{01}a_{00})$ or $(a_{00}a_{01})$. Putting

$$M(r,s) = 2\sum_{j=s-1}^{r+s-1}\binom{j}{s-1}\binom{k-2r-1}{j}\binom{k-r-j}{r-j+s-1}\binom{k-r-s}{R-s}\binom{n-k+r+s}{R} \tag{9}$$

then $A_{k,R}^{2,n}$ becomes

$$\begin{aligned} A_{k,R}^{2,n} &= \sum_{s=1}^{R}\sum_{r=0}^{[\frac{k}{2}]} M(r,s) \qquad \ldots \text{ for } k \text{ odd, and} \\ A_{k,R}^{2,n} &= \sum_{s=1}^{R}\sum_{r=0}^{\frac{k}{2}-1} M(r,s) + \binom{\frac{k}{2}-1}{R-1}\binom{n-\frac{k}{2}+1}{R} \quad \ldots \text{ for } k \text{ even.} \end{aligned} \tag{10}$$

The proof of the relations for $A_{k,R}^{2,n}$ is similar to that sketched for the special case $R = k$. Since, however, it is much longer, it is omitted here. Of course, eqn.(10) contains eqn.(8) as a special case.

2.2.2 Two linear chains (Hexagon)

For a double chain of $2n$ hexagons the application of results from combinatorics on words allows to derive a relation for $A_{k,R}^{2,n}$, the number of words of length n which possess – with the exception of the factor $(a_{10}a_{01})$ – the same $R-1$ factors as stated in the previous section:

$$A_{k,R}^{2,n} = \binom{k-1}{R-1}\cdot\sum_{j=[\frac{k-1}{2}]}^{k-1}\binom{k+1}{2(k-j)-1}\binom{n-j}{R} \tag{11}$$

Again, due to the limited space available, the proof of (11) is omitted.

2.2.3 m linear chains

So far, only a few exact results have been obtained for the $m \times n$-plane. This is due to the increased complexity of the problem. In terms of combinatorics on words the question to be answered is the following :

given an alphabet consisting of 2^m different letters $L_1, L_2, \ldots, L_{2^m}$, then, what is the number of words of length n that can be formed from these letters containing exactly j_{rs} factors $(L_r L_s)$, $1 \leq r, s \leq 2^m$, with $\sum_{r,s} j_{rs} = n - 1$?

For $m = 3$ (8 letters) these numbers have been calculated on a computer for lengths $n \leq 16$. Owing to computational difficulties (CPU-time, bulk of data to be analyzed) neither m nor n can be increased significantly so to be able to derive relations similar to those for $m = 1$ or 2. Therefore, according to our present state of knowledge, we believe that different approaches have to be taken in order to solve the problem of two colorings of the plane. Preliminary results show that Monte-Carlo-simulation seems to be the most promising approach to solve our problem.

Acknowledgement

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