20th International Conference
ENGINEERING MECHANICS 2014
Svratka, Czech Republic, 12 – 15 May 2014

REDUCING PERIODICITY IN MICROSTRUCTURE RECONSTRUCTION OF HETEROGENEOUS MATERIALS

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Abstract: *An approach to modelling of heterogeneous materials by means of Wang tilings is outlined in the paper. The presented tiling concept can be understood as an extension to the widely accepted Periodic Unit Cell (PUC) approach. Unlike in the case of PUC, the microstructural information is compressed within a set of Wang tiles instead of a single cell, which allows us to eliminate periodicity and efficiently control long range orientation orders of a microstructure reconstruction. In this contribution tile morphology design based on the automatic tile design is used. Further enhancement reducing the repetitiveness by microstructural patch is proposed. A sensitivity study of automatic design parameters is performed in order to preserve spatial features of original microstructure.*

Keywords: **Wang tilings, Microstructure compression and reconstruction, Automatic tile design, Patched tiles.**

1. Introduction

Driven by the economic competition and worldwide trend in energy efficiency it is vital for manufacturers to produce high performance materials at low cost (both in sense of price and energy consumption). Composite materials are generally recognized way to meet these requirements. A capable model that links the properties of individual phases and their composition with the overall behaviour is thus desired, thereby allowing for an efficient virtual design of the materials. A widely accepted approach of microstructure representation is based on the concept of Periodic Unit Cell (PUC), in which the microstructure is substituted with a single cell assumed to be periodically extended in appropriate spatial directions. From this point of view, the presented concept of Wang tilings can be understood as a generalization since the microstructural information is, contrary to PUC, attributed to a set of smaller domains denominated as Wang tiles. The tilings allow to overcome the periodic nature of reconstructed microstructures bear upon the PUC concept.

2. Wang Tilings

The concept is named in honour of Hao Wang, who, in 1961, presented his tiling as a method to prove the validity of a certain type of mathematical statements by converting it into a corresponding set of Wang tiles and solving the task whether the set can tile an infinite plane or not (Wang, 1961; Wang, 1965). Wang's fundamental premise that the infinite plane can be covered with tiling only periodically was disapproved by his student Robert Berger who discovered the first set allowing only for aperiodic planar tilings. This finding triggered a pursuit of the smallest aperiodic set (Grunbaum & Shephard, 1986). The smallest set discovered to date (as of 2014) contains 13 tiles and was presented by mathematician Karel Čulík (Culik II, 1996). These sets have been used e.g. in modelling of quasi-crystals (Aristoff & Radin, 2011) or DNA self-assembly structures (Winfree et al., 1998). The appealing feature of Wang tilings of producing naturally looking less repetitive textures was first reported by Stam (Stam, 1997). This application inspired our current research that brings the tiling concept to Materials Engineering community (Novák et al., 2012).

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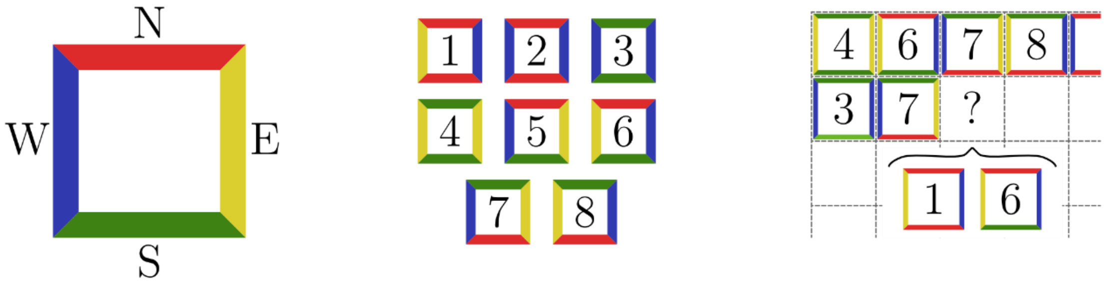
The basic element of the concept is a square dominoe-like[1] tile with codes assigned to its edges; in Fig. 1b represented with different colours. In general, the edges are usually referred to the corresponding cardinal directions as W-west, N-north, E-east and S-south. In a valid[2] tiling all tiles are placed in such a manner that the adjacent tiles have the same codes on the congruent edges.

For the purposes of the Materials Engineering (Novák et al., 2012) as well as Computer Graphics (Cohen et al., 2003) stochastic tile sets are preferred to their strictly aperiodic counterpart. Albeit not strictly aperiodic they give more freedom in choice of the number of codes and their spatial permutations around the tile perimeter. This particular feature together with the stochastic tiling algorithm (Cohen et al., 2003) make them correspond better to the intended use in modelling of materials with random microstructures.



a) *b)* *c)*

Fig. 1: Illustration of: a) Wang tile; b) Set of tiles W8/2-2; c) A step of stochastic tiling algorithm.

Reconstructed microstructure of arbitrary dimensions can be assembled from the given tiles by making use of the stochastic tiling algorithm proposed by Cohen et al. (2003). A regular tiling grid is filled with tiles in column-by-column, row-by-row order. In each loop, a subset of tiles satisfying edge constrains given by the previously placed tiles is filtered out of the tile set and a tile from the subset is randomly chosen and placed. The procedure is illustrated in Fig. 1c. To preserve the stochastic nature of the tiling yields the condition that at least a pair of tiles of each admissible NW edge code combination is present in the tile set.

3. Automatic Tile Design

Morphology of each tile, in the sense of the amount of microstructural information contained, has to be designed so that the reconstructed representation corresponds with the target system. Moreover, continuity of the morphology across the corresponding edges has to be guaranteed. Employing the optimization methods as reported by Novák et al. (2012) is general, however can be cumbersome from the computational efficiency point of view. Therefore, the automatic procedure proposed by Cohen et al. (2003), such as it makes the direct use of samples of reference microstructure, is reported in this work.

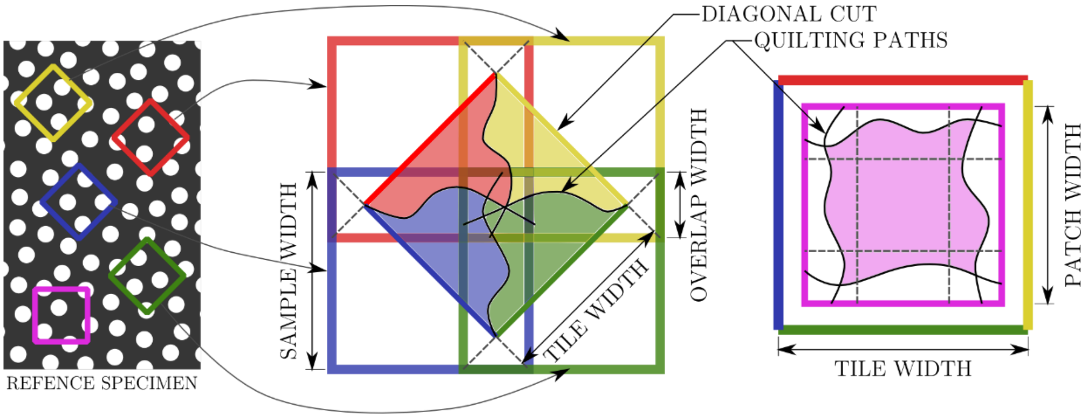
In brief, a number of samples is taken out from the given reference microstructure. Each sample corresponds to an edge code of the designed tile, which arises from the square cut-out of four partially overlapping samples positioned according to the desired edge code permutation, Fig. 2a. The diagonal cut through each sample ensures the compatibility of the microstructure morphology across the edges, assuming we store the remaining part for tiles involving opposite information. What remains is to fuse the samples in the overlap region without creating visible artefacts and errors in the morphology of the tile interior. For this purpose the Image Fusion algorithm (Efros & Freeman, 2001) modified to preserve inclusion shapes (Doškář, 2014) is used to locate a path along which the two samples are stitched together. In Fig. 2a, the path is highlighted in black. In order to split the microstructural information of the tile among edges and interiors, convenient from the viewpoint of spatial features of synthesized tilings, Novák et al. (2012), we further propose to stitch a patch to individual tiles as displayed in Fig. 2b.

The performance of the automatic tile design is governed by many parameters, width of the overlap region, dimension of the samples to be fused, and number of edge codes to name a few. Therefore, the sensitivity of results to those parameters was analysed for four reference microstructures, artificial and

[1] Alternatively called tetraminoe.

[2] Only valid tilings are assumed in the paper further on.

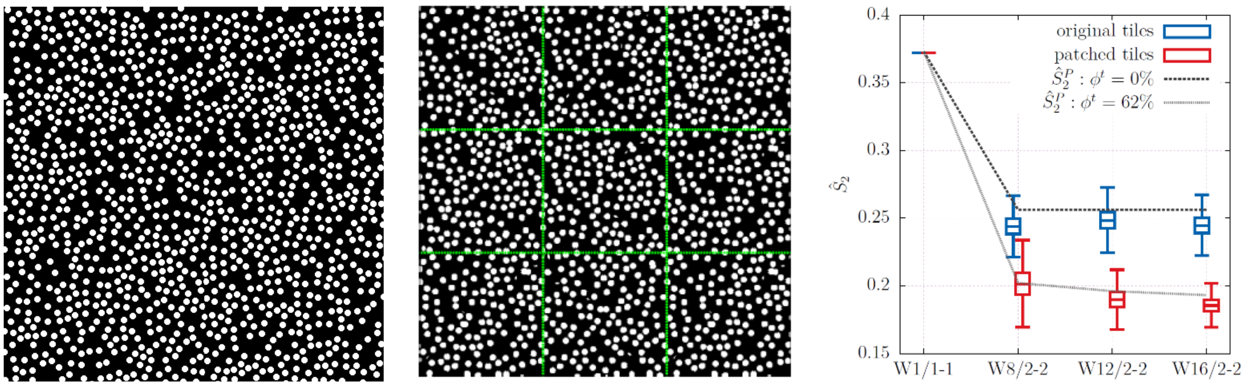
real. The proximity of reference and reconstructed media was quantified by means of spatial statistics. Namely, the volume fraction of phases, two-point probability and two-point cluster functions were calculated and compared.



a) *b)*

Fig. 2: Illustration of: a) Automatic tile design; b) Patch enhancement.

Based on this, the optimal width of the overlap region seems to be five to six times the mean the characteristic dimension of inclusions. Conversely, there seem not to exist a general rule for the number and dimension of the cut-outs; the same performance can be achieved either with smaller set of larger tiles or vice versa. The choice depends on a particular material composition or available computational resources. Therefore a similar analysis should be an integral part whenever a microstructure compression by making use of the tiling concept is planned.



a) *b)* *c)*

Fig. 3: Hard-disk monodispersion: a) Reference specimen; b) Reconstruction in 3x3 tiling; c)°Comparison of predicted and actual values of local extremes $\hat{S}_2$.

4. Quantification of Long Range Orientation Orders

As was mentioned, the main goal of this contribution lies in efficient microstructure representation along with the reduction of the repetitive nature of the reconstruction. The parasitic Long Range Orientation Orders (LRO) induced, were quantified by means of local extremes $\hat{S}_2$ in the two-point probability function $S_2(\boldsymbol{x})$. In the case of reconstructions based on PUC these take place at a distance of the PUC dimension and are of the same magnitude as at the origin, i.e. $\hat{S}_2^{PUC} = S_2(\mathbf{0})$. If the tiling concept is applied the local extremes are reduced within the bounds due to Novák et al. (2012):

$$\hat{S}_2^P \approx \frac{\Phi^t}{n^t}[\Phi + (n^t - 1)\Phi^2] + \max_i \left\{\frac{\Phi^e}{n_i^c}[\Phi + (n_i^c - 1)\Phi^2]\right\} \qquad (1)$$

The reduction is governed by number of tiles n^t, number of distinct edge codes n_i^c in the set and the portion of unique information attributed either to the tile interior or to the tile edges, described with Φ^t and Φ^e, respectively, such that it holds $\Phi^t + \Phi^e = 1$. Since there is the entire microstructural information attributed to edges when using the original automatic tile design, i.e. $\Phi^e = 1$, the magnitude of LRO depends solely on the number of edge codes. As the minimal stochastic set contains at least $n^t = 2n_1^c n_2^c$ tiles, adding edge codes leads to quadratic growth in number of tiles. Therefore the patched variant of the automatic tile design, presented in the previous section, seems the remedy as it allows for a significant reduction of LRO while keeping the number of tiles at feasible figures. On the other hand, patching requires additional inputs which raise demands on the quantity of reference microstructure samples. In Fig. 3 the comparison of the prediction given by Eq. (1) with the actual values of local extremes due to parasitic LRO is shown, namely for hard-disks monodispersion microstructure.

5. Conclusions

This contribution proposes a blend of techniques known in Discrete Mathematics (tiling), Computer Graphics (automatic tile design) and spatial statistics (sensitivity analysis) in order to build an efficient tool for microstructure compression and reconstruction. As shown in Fig. 3 employing the tiling concept significantly reduces the repetitive nature of the representation, especially when the patched tiles are used. Moreover, the automatic tile design is a faster alternative to optimization methods, time necessary to produce a tile set is of order of minutes. Note, that the automated processes can be also utilized to produce a Statistically Equivalent Periodic Unit Cell, the simplest Wang tile set W1/1-1. Despite the fact, that some guidance on design inputs is provided in the Section 3, to perform an analysis similar to the presented one is recommended whenever a microstructure is to be compressed via Wang tilings.

Besides the effective LRO control, the tiling concept proved to be a suitable way to model materials of which the Representative Volume Element dimensions are enormous, e.g. foams with high porosity, and cannot be effectively described by a single PUC (Doškář, 2014). Moreover, the potential of the tiling is further seen in evaluating the microstructure-informed enrichment functions for the Generalized Finite Element Methods (Novák et al., 2013).

Acknowledgement

The financial support by the Czech Science Foundation, grant No. 13-027024S (JN, MD), the European Social Fund, grant No. CZ.1.07/2.3.00/30.0005 "Creation of excellence interdisciplinary research teams at the Brno University of Technology" (JN), and the Grant Agency of the Czech Technical University in Prague, grant No. SGS14/028/OHK1/1T/11 "Modelling of random heterogeneous materials" (MD), are gratefully acknowledged.

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