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# Structure of micro-crack population and damage evolution in quasi-brittle media

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ABSTRACT

Mechanical behaviour of quasi-brittle materials, such as concrete and rock, is controlled by the generation and growth of micro-cracks. A 3D lattice model is used in this work for generating micro-crack populations. In the model, lattice sites signify solid-phase blocks and lattice bonds transmit forces and moments between adjacent sites. Micro-cracks are generated at the interfaces between solid-phase blocks, where initial defects are allocated according to given size distribution. This is represented by removal of bonds when a criterion based on local forces and defect size is met. The growing population of micro-cracks results in a non-linear stress–strain response, which can be characterised by a standard damage parameter. This population is analysed using a graph-theoretical approach, where graph nodes represent failed faces and graph edges connect neighbouring failed faces, i.e. coalesced micro-cracks. The evolving structure of the graph components is presented and linked to the emergent non-linear behaviour and damage. The results provide new insights into the relation between the topological structure of the population of micro-cracks and the material macroscopic response. The study is focused on concrete, for which defect sizes were available, but the proposed methodology is applicable to a range of quasi-brittle materials with similar dominant damage mechanisms.


## 1. Introduction

The mechanical behaviour of quasi-brittle materials, such as concrete, graphite, ceramics, or rock, emerges from underlying microstructure changes. The meaning of microstructure differs for different media and could be characterised by intrinsic length scales. For concrete these could be aggregate sizes and inter-aggregate distances, while for rock systems these could be sizes of blocks formed between existing small fractures. At the engineering length scale, orders of magnitude larger than the microstructure scales, the mechanical behaviour can be described with continuum constitutive laws of increasing complexity combining damage, plasticity and time-dependent effects [1–4]. In these phenomenological approaches damage represents reduction of the material elastic constants. From microstructure length scale perspective damage in quasi-brittle media is introduced by nucleation and evolution of micro-cracks, where a micro-crack means a fracture of the order of the microstructure scale(s). Potentially the effect of the micro-cracks formed under loading could be captured by continuum damage models calibrated against engineering scale experiments. The phenomenology, however, cannot help to understand the effects of the generated micro-crack population on other important physical properties of the material. In many applications the quasi-brittle materials have additional functions as barriers to fluid transport via convection, advection, and/or diffusion. It is therefore important to take a mechanistic view on the development of damage by modelling the evolution of micro-crack population. This can inform us about changes in the transport properties. Such a mechanistic approach needs to account for the microstructure in a way corresponding to the micro-crack formation mechanism [5]. In concrete, micro-cracks typically emerge from pores in the interfacial transition zone between the cement paste and aggregates [6]. In rock systems, micro-crack generating features could be existing fractures as well as pores. Concrete will be used in this work to demonstrate the proposed methodology, because data for the micro-crack initiating features in this material is readily available.

Discrete lattice representation of the material microstructure seems to offer the most appropriate modelling strategy for analysis of micro-crack populations. Discrete lattices allow for studies of distributed damage without constitutive assumptions about crack paths and coalescence that would be needed in a continuum finite element modelling. For lattice construction, the material is

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appropriately subdivided into cells and lattice sites are placed at the cell centres. The deformation of the represented continuum arises from interactions between the lattice sites. These involve forces resisting relative displacements and moments resisting relative rotations between sites. Two conceptually similar approaches have been proposed to link local interactions to continuum response. In the first one, the local forces are related to the stresses in the continuum cell, e.g. [7,8]. In the second one, the interactions are represented by structural beam elements, the stiffness coefficients of which are determined by equating the strain energy in the discrete and the continuum cell, e.g. [9,10]. In both cases explicit relations between local and continuum parameters can be established for regular lattices. It has been previously shown that regular 3D lattices based on simple cubic, face-centred cubic and hexagonal closely-packed atomic arrangements can be used to represent materials exhibiting cubic elasticity. However, the only isotropic materials such lattices could represent are materials with zero Poisson's ratio [11].

A bi-regular lattice that can represent all materials of practical interest has been proposed recently [12]. It can be seen as a lattice based on body-centred cubic atomic arrangement with two types of links - between neighbours along body diagonals (nearer) and between neighbours along cell edges (further). This lattice, currently formed by beams clamped at sites, is used in the current work together with microstructure data for concrete obtained with X-ray computed tomography. Failure models based on microstructure data and the novel lattice have been previously used for modelling tensile and compressive behaviour of cement [13] and the compressive behaviour of concrete under various complex loading conditions [14]. This work makes a step into developing our understanding of the micro-crack population and its relation to macroscopic damage. Further, the structure of the micro-crack population will provide the means to study the changes in transport properties with damage in future studies.

Most of the work relating micro-crack populations to elastic moduli follows the fundamental paper [15], where analytical statistical derivation of the relation was provided. We follow the interpretation given in [16], in which the damage is measured as a relative change of the elastic modulus and related to micro-crack population via

$$D = 1 - \frac{E}{E(0)} = \frac{\beta}{N_T}\sum_{c\geq 1} c^3 N(c), \tag{1}$$

where $c$ is some measure of micro-crack size, $N(c)$ is the number of micro-cracks of size $c$, $N_T$ is the total number of sites capable of nucleating micro-cracks, and $\beta$ is a scaling parameter reported as $0.47\pi$ for cracks in a 2D medium. Eq. (1) is our point of comparison for the simulations performed with the lattice model for various loading cases. In the current work we are interested in testing the range of applicability of Eq. (1) and understanding the reasons for deviation from this rule, should such occur, by explicitly analysing the micro-crack population growth. It should be mentioned, that we do not presuppose a value for the scaling parameter $\beta$. The simulations are performed with a 3D model and used to derive mechanistically relations between mechanical damage parameters and geometrical characteristics of formed micro-crack populations. The scaling parameter $\beta$ could be extracted from such relations only for special loading cases as shown in Section 4.

## 2. Materials and methods

### 2.1. The site-bond model

The lattice model used in this work is illustrated in Fig. 1. The unit cell, shown in Fig. 1(a) is a truncated octahedron – a solid with six square and eight regular hexagonal boundaries. The 3D space can be compactly tessellated using such cells, with each cell representing a material microstructure feature, e.g. a block or a grain, in an average sense. This representation is supported by physical and statistical arguments [12]. In brief, the truncated octahedron is topologically closest to the average cell in a random Voronoi subdivision of space. A discrete lattice is formed by placing sites at the centres of the cells and connecting each site to its 14 nearest neighbours; example is shown in Fig. 1(b). The lattice contains two types of bonds. Bonds denoted by $B_1$ are normal to the square boundaries and form an orthogonal set. For convenience this set is made coincident with the global coordinate system and $B_1$ are referred to as the principal bonds. Bonds denoted by $B_2$ are normal to the hexagonal boundaries. The hexagons lie on the octahedral planes with respect to the selected coordinate system, hence $B_2$ are referred to as the octahedral bonds.

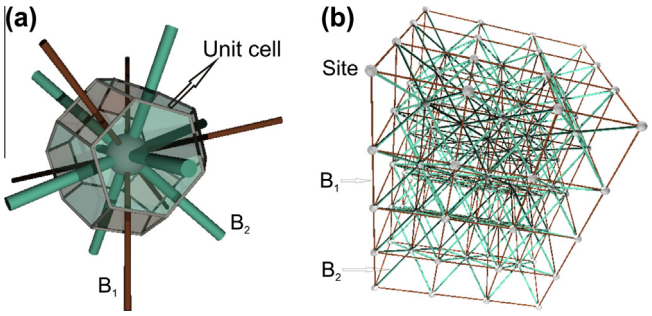


**Fig. 1.** Lattice illustration: (a) unit cell showing the site with 14 coordinating bonds: six principal, $B_1$, and eight octahedral, $B_2$ and (b) discrete lattice of beam elements.

If the spacing between sites in the principal directions is denoted by $L$, bonds $B_1$ have length $L_1 = L$, and bonds $B_2$ have length $L_2 = \sqrt{3}\,L/2$. Presently, the bonds are represented by structural beam elements of circular cross sections, with $R_1$ and $R_2$ denoting the radii of beams $B_1$ and $B_2$, respectively. The beams are clamped at the lattice sites. The two types of beams have identical Young's modulus, $E_b$, and Poisson's ratio, $\nu_b$. This reflects the understanding that locally, i.e. at a cell length scale, the material is homogeneous. It has been previously shown [12], that by calibrating four parameters: $R_1/L$, $R_2/L$, $E_b$, and $\nu_b$, the lattice can produce any material with cubic elasticity and with special selections a large class of isotropic elastic materials with Poisson's ratios of practical interest. The reference material in this work is a concrete with $E = 46$ GPa and $\nu = 0.27$, for which the calibration, assuming isotropic elasticity, yields $R_1/L = 0.2$; $R_2/L = 0.32$; $E_b = 90$ GPa; and $\nu_b = 0.4$ [14]. The commercial software Abaqus [17] with Euler–Bernoulli beam formulation has been used for the calibration and the analyses reported in this work.

### 2.2. Pore distribution and model length scale

Microstructure data for the reference material was obtained using X-ray Computed Tomography as reported in [14]. The pore size distribution was obtained by segmentation of reconstructed 3D images. The studied regions of interest had dimensions of $1700 \times 1200 \times 1200$ voxels with a voxel size of ca. 15 μm, allowing for a minimum detectable pore radius of ca. 15 μm. The number of pores measured experimentally was $n \approx 41{,}500$. The measured pore radii, $c_i$, were used to construct a cumulative probability distribution (CPD) with standard median ranking, where for pore radii ordered as $c_1 \leqslant c_2 \leqslant \cdots \leqslant c_n$, the cumulative probability for pores with radii less than $c_i$ is given by $F(c < c_i) = (i - 0.3)/(n + 0.4)$. The CPD for the reference material is shown in Fig. 2(a), where the

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