

# LATTICE MODELING OF FRACTURE PROCESSES IN NUMERICAL CONCRETE WITH IRREGULAR SHAPE AGGREGATES

ZHIWEI QIAN<sup>\*</sup> AND ERIK SCHLANGEN<sup>†</sup>

<sup>\*</sup> Materials innovation institute M2i  
Delft University of Technology  
Delft, the Netherlands  
e-mail: z.qian@tudelft.nl, www.m2i.nl

<sup>†</sup> Delft University of Technology  
Delft, the Netherlands  
e-mail: h.e.j.g.schlangen@tudelft.nl, www.microlab.citg.tudelft.nl

**Key words:** Lattice Model, Concrete Fracture, Irregular Shape Aggregates

**Abstract:** The fracture processes in concrete can be simulated by lattice fracture model [1]. A lattice network is usually constructed on top of the material structure of concrete, and then the mechanical properties of lattice elements are assigned, corresponding with the phases they represent. The material structure of concrete can be obtained experimentally by X-ray computed tomography. Alternatively it is also possible to simulate a virtual material structure of concrete. A simple way to represent the material structure of concrete is to put multiple spheres in a matrix, where the spheres are interpreted as aggregates. This assumption of the shape of aggregates might have influences on the fracture processes in concrete, such as the microcracks propagation path.

Recently the Anm material model was proposed and implemented, which can produce a material structure of concrete with irregular shape aggregates [2]. The irregular shape is represented by a series of spherical harmonic coefficients. The method to determine these spherical harmonic coefficients from aggregate shapes was elaborated in [3]. The further mechanical performance evaluation would benefit from this more realistic material structure.

In this paper a material structure of concrete is simulated by the Anm material model. A number of irregular shape particles are planted in a matrix. This material structure is then converted into a voxelized image. Afterwards a random lattice mesh is made, and three types of lattice elements are defined, which represent aggregates, matrix and interface respectively. A uniaxial tensile test is set up and simulated by fixing all the lattice nodes at the bottom of the specimen and imposing a prescribed unit displacement onto all the nodes at the top. The lattice fracture analysis gives the stress-strain response and microcracks propagation, from which some mechanical properties such as Young's modulus, tensile strength and fracture energy can be predicted.

## 1 INTRODUCTION

Numerical modeling of fracture processes in brittle materials, such as cement paste, mortar, concrete and rocks, started in the late 1960s with the landmark papers of Ngo and

Scordelis [4] and Rashid [5], in which the discrete and smeared crack models were introduced. Especially the latter approach gained much popularity, and in the 1970s comprehensive efforts were invested in

developing constitutive models in a smeared setting which could reproduce the experimentally observed stress-strain characteristics of concrete. However, neither of them could tell the fracture processes in detail. In the 1990s, Schlangen and van Mier proposed another model to compensate the drawbacks of discrete and smeared crack models, which is called lattice fracture model [1].

The concept of lattice was proposed by Hrennikoff in the 1940s to solve elasticity problems using the framework method [6]. In the 1970s and 1980s the lattice model was introduced in theoretical physics to study the fracture behavior of disordered media [7~8]. In the field of material sciences, a model was proposed by Burt and Dougill to simulate uniaxial extension tests, which consists of a plane pin-jointed random network structure of linear elastic brittle members having a range of different strengths and stiffnesses [9].

In the last two decades, plenty of efforts have been made to develop the lattice fracture model in a variety of different settings: regular / irregular network, triangular / quadrangular mesh, truss / beam element, the way to implement heterogeneity (random distribution of local properties / microstructure mapping) and whether to introduce the softening at the element level. A lattice system of truss elements was constructed based on a random particle model to study the fracture of aggregate or fiber composites by Bazant et al. [10]. The tension softening response of the matrix phase was implemented in the lattice fracture analysis for concrete by Arslan et al. [11]. The fracture of particle composites due to large deformation was investigated by Karihaloo et al. using lattice fracture model [12]. Vervuurt made use of lattice fracture analysis to study the interface fracture in concrete [13], and van Vliet investigated the size effect in tensile fracture of concrete and rock [14]. The size effect on strength in numerical concrete was also studied by Man, where the influences of aggregate density and shape were discussed [15]. An irregular lattice model was proposed by Bolander and Sukumar for simulating quasistatic fracture in

softening materials, in which accurate modeling of heterogeneity is enabled by constructing the lattice geometry on the basis of a Voronoi discretization of the material domain [16]. Lattice modeling of uniaxial compression was studied and applied to normal concrete, high strength concrete and foamed cement by Caduff and van Mier [17]. Grassl and Davies modeled corrosion induced cracking and bond in reinforced concrete using lattice approach [18]. Fracture laws for simulating compressive fracture in lattice-type models were explored and discussed by van Mier [19]. The possibility of modeling self-healing of cementitious materials using lattice approach was investigated by Joseph [20].

In the lattice fracture model, the continuum is replaced by a lattice of beam elements. Subsequently, the microstructure of the material can be mapped onto these beam elements by assigning them different properties, depending on whether the beam element represents a grain or matrix. Various conventional laboratory experiments like uniaxial tensile test, compressive test, shear test, bending test and torsional test can be simulated by the lattice fracture model and the model can be applied towards a wide range of multiphase materials, such as concrete [21], cement paste [22], graphite and fiber reinforced concrete [23].

The lattice fracture model can solve both 2D and 3D problems as the principles are the same. The differences mainly exist in the computational resources requirements in terms of computer memory and computing time. Hence comprehensive efforts were made to reduce the memory demand by employing a matrix free linear algebraic equation solver [24]. The pre-conditioned conjugate gradient algorithm is also applied to guarantee the convergence of solutions to linear equations resulting from very large size lattice structure. Parallel computing for lattice fracture analysis is a good solution to save computational time and be able to analyze even larger lattice structure [25]. A parallel computer implementation of lattice fracture model for shared memory architecture computers was developed by Qian et al. in 2009, in which

OpenMP API (Application Program Interface) was used in combination with the host programming language C++.

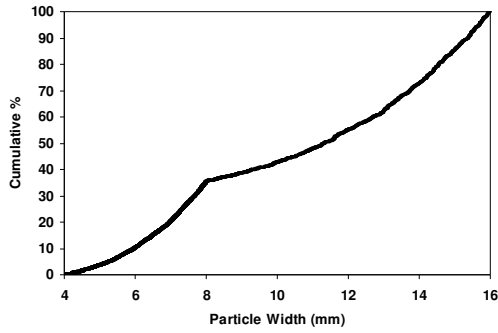
A lattice network is usually constructed on top of the material structure of concrete, and then the mechanical properties of lattice elements are assigned, corresponding with the phases they represent. The material structure of concrete can be simulated by the Anm material model, which can produce a material structure of concrete with irregular shape aggregates [2]. The irregular shape is represented by a series of spherical harmonic coefficients. The method to determine these spherical harmonic coefficients from aggregate shapes was elaborated in [3]. The further mechanical performance evaluation would benefit from this more realistic material structure.

## 2 SIMULATION OF NUMERICAL CONCRETE WITH IRREGULAR AGGREGATES

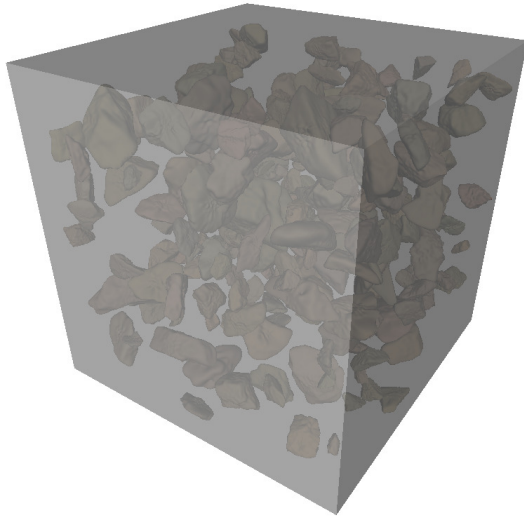
In the Anm material model, the concept of particles embedded in matrix applies. An empty container is created to represent a specimen at the beginning, and then all the particles are placed one after another into this container, from the larger ones to smaller ones. It is good to start with the largest particles as it would be more difficult to place them if they were processed at a later stage. All the particles are separated into several sieve ranges according to the particle sizes indicated by the particle widths. The largest sieve range is processed first, a width within this sieve range is picked randomly and assigned to a particle which is chosen from the appropriate particle shape database. The particle shape database can be created for varying classes of powders and aggregates with the procedures proposed in [3]. An arbitrary rotation is performed on the particle to get rid of possible orientation bias, which might be introduced during the production of the particle shape database. After the rotation the particle is placed at a randomly chosen primary location in the specimen, and then the ghost locations are determined if any, depending on the type

of the specimen boundary conditions and the position of the particle. The primary particle and its ghost particles are checked against all the previously placed particles for overlap. If no overlap is detected, then the particle enters the simulation box successfully, otherwise it will be moved to a new randomly chosen location. The reassignment of the location is subject to a pre-defined maximum number of attempts. After the consecutive failures reach the limit, the particle will be resized to another randomly selected width within the current sieve range, and then be thrown into the specimen following the same trial-and-error procedure. The particle size rescale is also subject to a pre-defined maximum number of attempts. If the rescales do not help, then the particle will be rotated again to have another orientation. If the problem still exists, then a new shape will be chosen from the particle shape database. In case the particle cannot find its position eventually, it may suggest there is no space available for new particles within the current sieve range. The next sieve range will be processed if no availability for the current sieve range is found, or all the particles within the current sieve range have already been placed. The above trial-and-error procedure is called parking procedure and it is the essential of the Anm material model.

Concrete specimen of the size 150 mm in the cubic shape is simulated by the Anm material model. The specimen has two phases, the mortar matrix and crushed stone aggregates. Non-periodic material boundary applies, which requires all the particles are inside the specimen and no part of a particle can pass through a surface. The total mass of the crushed stones is 2653 g, and 64% of which are in the sieve 8~16 mm, the rest 36% are in the sieve 4~8 mm. The particle size is taken as the particle width and its distribution for the coarse aggregates is given in [Figure 1](#). The volume percentage of the crushed stones in the concrete specimen is 30%. The simulated mesostructure of the concrete specimen with irregular shape crushed stones is sketched in [Figure 2](#).



**Figure 1:** Particle size distribution for the coarse aggregates in concrete



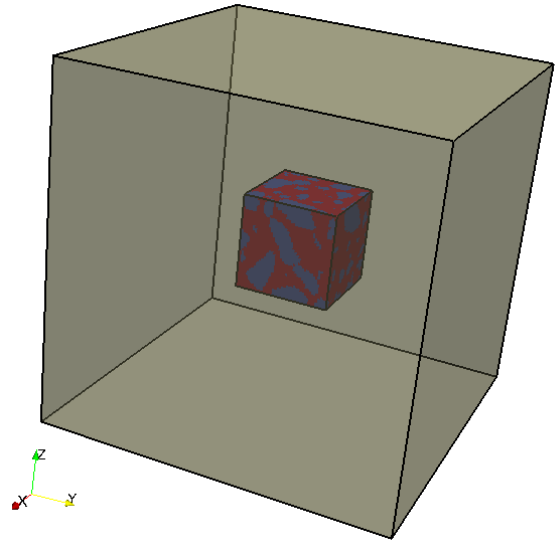
**Figure 2:** The mesostructure of the concrete specimen with irregular shape crushed stones

### 3 MECHANICAL PERFORMANCE EVALUATION

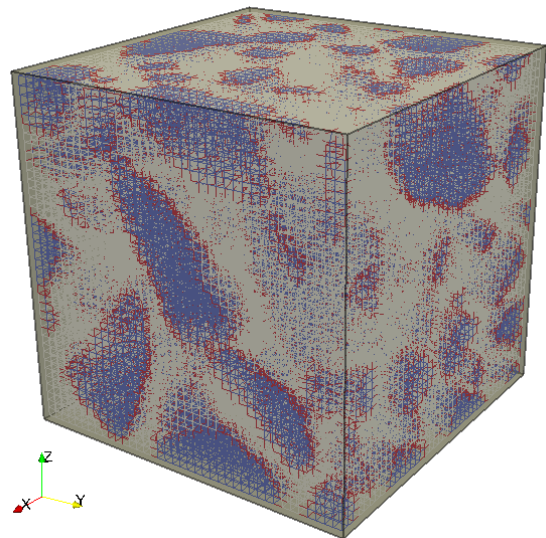
The mechanical performance of the numerical concrete specimen in the previous section can be evaluated by simulating a uniaxial tensile test on it using the lattice fracture model.

To reduce the computational effect, a smaller specimen of the size 40 mm is cut out from the original 150 mm specimen at its center, as shown in Figure 3. The 40 mm concrete specimen is then digitized at the resolution of 1 mm, and consists of two solid phases namely stone and mortar. A lattice network is constructed based on the digital concrete specimen, and three types of lattice

elements are identified, which represent crushed stone, mortar and interface respectively, as shown in Figure 4. The local mechanical properties are given in Table 1. The properties of the lattice elements representing mortar are varied randomly to reflect the heterogeneity of mortar phase.



**Figure 3:** 40 mm out of 150 mm concrete specimen at its center

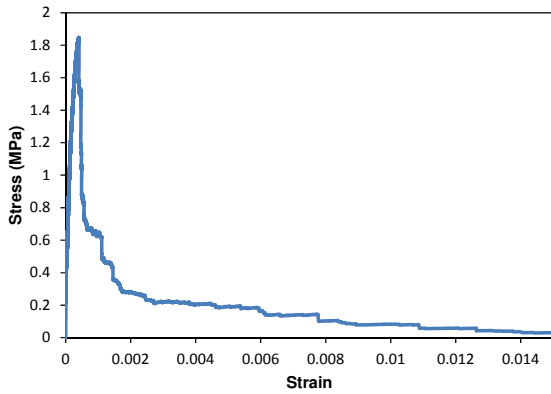


**Figure 4:** Lattice mesh of the 40 mm concrete specimen

**Table 1:** Local mechanical properties of stone, mortar and interface elements in concrete

	Young's modulus (GPa)	Tensile strength (MPa)
Stone	70	24
Mortar	17~65	1.1~19.5
Interface	41	1

A uniaxial tensile test is simulated on the lattice system meshed from the 40 mm concrete specimen as shown in [Figure 4](#), using the local mechanical properties listed in [Table 1](#). The resulting stress-strain response is presented in [Figure 5](#), and some mechanical properties can be computed as given in [Table 2](#).

**Figure 5:** Simulated stress-strain response of the 40 mm concrete specimen**Table 2:** Simulated mechanical properties of the 40 mm concrete specimen

Young's modulus (GPa)	Tensile strength (MPa)	Strain at peak load	Fracture energy ( $J/m^2$ )
31	1.8	0.04%	127

The pattern of the simulated stress-strain response of the 40 mm concrete specimen is similar to the one observed in laboratory, and the mechanical properties computed from the stress-strain diagram are also located within the reasonable range.

## 4 SUMMARY

In this paper a material structure of concrete is simulated by the Anm material model. A number of irregular shape particles are planted in a matrix. This material structure is then converted into a voxelized image. Afterwards a random lattice mesh is made, and three types of lattice elements are defined, which represent aggregates, matrix and interface respectively. A uniaxial tensile test is set up and simulated by fixing all the lattice nodes at the bottom of the specimen and imposing a prescribed unit displacement onto all the nodes at the top. The lattice fracture analysis gives the stress-strain response and microcracks propagation, from which some mechanical properties such as Young's modulus, tensile strength and fracture energy can be predicted.

## ACKNOWLEDGEMENTS

This research was carried out under project number M83.1.12459 in the framework of the Research Program of the Materials innovation institute M2i (<http://www.m2i.nl>). Part of this work was sponsored by the European Union FP7 project CODICE (<http://www.codice-project.eu>).

## REFERENCES

- [1] Schlangen, E. & van Mier, J., Experimental and numerical analysis of micromechanisms of fracture of cement-based composites, *Cement and Concrete Composites*, 1992, **14**, 105-118
- [2] Qian, Z., Multiscale Modeling of Fracture Processes in Cementitious Materials, PhD thesis, Delft University of Technology, 2012
- [3] Garboczi, E., Three-dimensional mathematical analysis of particle shape using X-ray tomography and spherical harmonics: Application to aggregates used in concrete, *Cement and Concrete Research*, 2002, **32**, 1621-1638
- [4] Ngo, D. & Scordelis, A., Finite Element Analysis of Reinforced Concrete Beams, *J*

*Am Concr Inst*, 1967, **64**, 152-163

- [5] Rashid, Y., Ultimate strength analysis of prestressed concrete pressure vessels, *Nuclear Engineering and Design*, 1968, **7**, 334-344
- [6] Hrennikoff, A., Solution of problems of elasticity by the framework method, *Journal of Applied Mechanics*, 1941, **8**, 169-175
- [7] Ziman, J. M., Models of disorder: the theoretical physics of homogeneously disordered systems, Cambridge University Press, 1979
- [8] Herrmann, H. J.; Hansen, A. & Roux, S., Fracture of disordered, elastic lattices in two dimensions, *Phys. Rev. B*, American Physical Society, 1989, **39**, 637-648
- [9] Burt, N. J. & Dougill, J. W., Progressive Failure in a Model Heterogeneous Medium, *Journal of the Engineering Mechanics Division*, 1977, **103**, 365-376
- [10] Bazant, Z. P.; Tabbara, M. R.; Kazemi, M. T. & Pijaudier-Cabot, G., Random Particle Model for Fracture of Aggregate or Fiber Composites, *Journal of Engineering Mechanics*, 1990, **116**, 1686-1705
- [11] Arslan, A.; Ince, R. & Karihaloo, B., Improved Lattice Model for Concrete, *Fracture J. Eng. Mech.*, 2002, **128**, 57-65
- [12] Karihaloo, B.; Shao, P. & Xiao, Q., Lattice modelling of the failure of particle composites, *Engineering Fracture Mechanics*, 2003, **70**, 2385-2406
- [13] Vervuurt, A., Interface fracture in concrete, PhD thesis, Delft University of Technology, 1997
- [14] van Vliet, M. R., Size effect in tensile fracture of concrete and rock, PhD thesis, Delft University of Technology, 2000
- [15] Man, H.-K., Analysis of 3D scale and size effects in numerical concrete, PhD thesis, ETH Zurich, 2010
- [16] Bolander, J. & Sukumar, N., Irregular lattice model for quasistatic crack propagation, *Phys. Rev. B*, American Physical Society, 2005, **71**, 094106
- [17] Caduff, D. & van Mier, J. G., Analysis of compressive fracture of three different concretes by means of 3D-digital image correlation and vacuum impregnation, *Cement and Concrete Composites*, 2010, **32**, 281-290
- [18] Grassl, P. & Davies, T., Lattice modelling of corrosion induced cracking and bond in reinforced concrete, *Cement and Concrete Composites*, 2011, **33**, 918-924
- [19] van Mier, J. G., Fracture Laws for Simulating Compressive Fracture in Lattice-Type Models, *Materials Science Forum*, 2012, **706-709**, 1550-1555
- [20] Joseph, C., Experimental and Numerical Study of the Fracture and Self-healing of Cementitious Materials, PhD thesis, Cardiff University, 2008
- [21] Schlangen, E., Experimental and Numerical Analysis of Fracture Processes in Concrete, PhD thesis, Delft University of Technology, 1993
- [22] Qian, Z.; Schlangen, E.; Ye, G. & van Breugel, K., Prediction of Mechanical Properties of Cement Paste at Microscale, *Materiales de Construcción*, 2010, **60**, 7-18
- [23] Schlangen, E. & Qian, Z., 3D modeling of fracture in cement-based materials, *Journal of Multiscale Modelling*, 2009, **1**, 245-261
- [24] Schlangen, E. & Garboczi, E., Fracture simulations of concrete using lattice

models: Computational aspects,  
*Engineering Fracture Mechanics*, 1997,  
**57**, 319-332

- [25] Qian, Z.; Schlangen, E.; Ye, G. & van Breugel, K., Topping, B. & Ivanyi, P. (Eds.) Parallel implementation of three-dimensional lattice fracture analysis on a distributed memory architecture, *Proceedings of the First International Conference on Parallel, Distributed and Grid Computing for Engineering*, Civil-Comp Press, Stirlingshire, Scotland, 2009