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A mathematical model for plasticity and damage: A discrete calculus formulation

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ABSTRACT

In this article we propose a discrete lattice model to simulate the elastic, plastic and failure behaviour of isotropic materials. Focus is given on the mathematical derivation of the lattice elements, nodes and edges, in the presence of plastic deformations and damage, i.e. stiffness degradation. By using discrete calculus and introducing non-local potential for plasticity, a force-based approach, we provide a matrix formulation necessary for software implementation. The output is a non-linear system with allowance for elasticity, plasticity and damage in lattices. This is the key tool for explicit analysis of micro-crack generation and population growth in plastically deforming metals, leading to macroscopic degradation of their mechanical properties and fitness for service. An illustrative example, analysing a local region of a node, is given to demonstrate the system performance.

1. Introduction

Lattice models for analysis of deformation and fracture of solids have been developed over the last thirty years mainly for quasi-brittle materials, such as concretes and rocks [1,2], where local behaviour is elastic-brittle, i.e. the only mechanism for energy dissipation is the generation of new surfaces (brittle micro-cracking). Lattice models contain set of sites connected by bonds; in the language of algebraic topology this is a 1-complex embedded in $\mathbb{R}^2$ or $\mathbb{R}^3$, i.e. 2D or 3D graphs. The challenge with lattices is that they intend to represent a *continuous* solid by a discrete system. Specifically, the stored energy in any lattice region is required to be equivalent to the stored energy in the corresponding continuum region. This is used to derive a link between properties of lattice elements, e.g. bond stiffness coefficients, and macroscopic properties of the material. The macroscopic properties are experimentally measurable constants of the generalized Hook's law relating the stress and strain tensors. In the most general case, referred to as anisotropic, there are 21 independent constants due to the symmetry of the stress and strain tensors. However, most materials possess additional symmetries, which reduce the number of independent constants, e.g. orthotropic materials have nine constants and their properties differ in three perpendicular directions. This is typical for some ordered composites. Most common are the isotropic materials, including metallic and quasi-brittle, where the measurable properties are the same in all directions. These require only two constants to relate stresses to

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strains, e.g. elastic modulus and Poisson's ratio. Therefore linking properties of lattice elements to the constants of isotropic materials is of primary interest and utility. For irregular graphs this is not possible exactly; approximate calibrations of lattice properties for known macroscopic properties are used, e.g. [3]. For graphs with some regularity, the link can be established rigorously. For example, isotropic materials can be represented exactly by 2D graphs based on hexagonal structure, e.g. [4], and by 3D graphs based on truncated octahedral structure [5]. Other possible regular 3D graphs can represent cubic elasticity, i.e. three parameter elastic behaviour, but not isotropic elasticity, i.e. two parameter behaviour, typical for most engineering materials [6]. Nevertheless, lattices are being used because of the need to represent failure in materials, albeit not always with exactly calibrated local properties. Failure is a generation of a new internal surface, i.e. a non-topological concept. Hence, the classical continuum mechanics does not work, as it is a thermodynamic *bulk* theory.

Our work addresses cleavage fracture, which is a phenomenon of fast and catastrophic crack propagation. It can be observed in all metals with body-centred cubic crystal lattices due to the smaller number of slip planes, i.e. reduced ability to dissipate energy by plastic deformation. We are specifically interested in ferritic steels, used for example to manufacture nuclear reactor pressure vessels, where cleavage is a potential cause for serious concern. Cleavage is known to be triggered by rupturing of brittle second-phase particles, such as carbides, which typically decorate the grain boundaries of the polycrystal and can rupture due to plastic overload from the surrounding grains. The existing modelling of this phenomenon, the so called local approach to cleavage fracture, is based on the weakest-link statistic, i.e. global failure probability derives from the failure probabilities of individual particles, following prescribed size distribution but treated as independent events [7]. This approach works well for predicting cleavage fracture at very low temperatures, where plasticity is limited, the number of micro-cracks formed prior to cleavage is small and they are spatially scattered, i.e. only a set of largest particles failed. The probability of cleavage fracture, however, decreases rapidly with the increase of temperature, where plasticity is enhanced. This apparent increase of material toughness with temperature cannot be captured with the existing modelling strategy, despite of the many improvements in the particle rapture criterion over the years [8,9]. However, accurate assessment with reduced conservatism is needed for more economic exploitation of reactors, including better planning of inspection intervals and life-extension decisions. From the current status of modelling it can be deduced that the plasticity enhancement with temperature leads to generation of increasingly large micro-crack populations, in which case the argument behind the weakest-link statistic is violated, e.g. there is a significant effect of micro-crack interactions prior to ultimate cleavage. This will explain the reduced probability of cleavage, hence increased toughness, of the material with temperature. Lattice models are particularly suitable to study the generation and interaction of micro-cracks as they grow, coalesce and progress to final failure. To this end we present a lattice development relevant to plastically deforming metals.

A mathematically rigorous treatment of lattices can be achieved when they are analysed as graphs [10]. However, the discrete exterior calculus (DEC) specialized to graphs in this reference, is developed for scalar problems. This means that the nodal unknown (a 0-cochain) is scalar, i.e. temperature, pressure, concentration, etc. The gradient of this is also a scalar field over the edges (1-cochain). Things go relatively simply for such physical problems. In mechanics this approach is rather more difficult as we have a vector-valued nodal field, namely a displacement vector assigned to each node. Article [11] is the only one to our knowledge which attempts to apply DEC to mechanical problems in elastic settings. Our aim is to build upon this theoretical basis and present a graph-theoretical approach to lattices including elastic, plastic and damage behaviour.

Microstructure representation

Micro-structures of metals and alloys develop by a crystallization process, which starts at spatially randomly distributed nuclei and finishes when neighbouring growing crystals touch each other to form grain boundaries [12]. Under uniform temperature distribution, the individual crystals grow with equal rates and therefore the final micro-structure is described by the Voronoi diagram constructed around the set of nuclei [13]. The 3D Voronoi diagram is constructed by the intersection of planes bisecting normally the segments connecting each pair of neighbouring nuclei, as illustrated in Fig. 1. Thus, each crystal is a polyhedron representing the neighbourhood of a nucleus, where all points are closer to the nucleus than to any other nucleus. Initially, we seek to represent the poly-crystal with a regular tessellation of the 3D space, shown in Fig. 2, where a grain is topologically equivalent to the average grain in arbitrary Voronoi tessellation [14,15]. This simplifies the geometry and allows for exact calibration of the lattice emerging from the tessellation [5].

Cell complexes and their duals

Irrespective of whether we use an irregular tessellation of space (Voronoi around nuclei) or the regular tessellation of Fig. 2, the material is subdivided into compactly packed and non-intrusive 3D cells. Using terminology from algebraic topology, see [16], the polycrystal is a p-complex, where $p = 3$ embedded in $\mathbb{R}^d$, where $d = 3$. Thus, each crystal is a 3-cell, bounded by a number of 2-cells (planar polygonal faces), each of which is bounded by a number of 1-cells (edges), each of which is bounded by two 0-cells (nodes). It should be noted that $p = d$ is not a requirement for p-complexes embedded in $\mathbb{R}^d$; p-complexes with $1 \leq p \leq d$ can be formed and treated similarly. For example, the collection of all faces of the regularized polycrystal (or grain boundaries of the real microstructure) without the cell (grain) interiors is a 2-complex embedded in $\mathbb{R}^3$. It contains 0-cells, the vertices of the truncated octahedrons (or quadruple points in the real microstructure), 1-cells, the edges of the truncated octahedrons (or triple lines), and 2-cells, the faces of the truncated octahedrons (or grain boundaries). The structure of thin-walled closed cell foam can be viewed as a 2-complex. Similarly, the collection of all edges of the regularized polycrystal (or triple lines in the real microstructure) without the cell (grain) interiors and faces (boundaries) is a 1-complex embedded in $\mathbb{R}^3$. It contains 0-cells, the vertices of the truncated octahedrons (or quadruple points in the real microstructure), and 1-cells, the edges of the truncated octahedrons (or triple lines). The structure of thin-ligament open