Computer-Aided Design 97 (2018) 1–14

Contents lists available at ScienceDirect

Computer-Aided Design

journal homepage: www.elsevier.com/locate/cad

Integrated approach for geometric modeling and interactive visual analysis of grain structures☆

André Montes Rodrigues [a,*], Fernando Bardella [b], Marcelo Knorich Zuffo [a], Ricardo Mendes Leal Neto [b]

[a] Polytechnic School, Electronic Systems Department, University of São Paulo, 380 Prof. Luciano Gualberto Av, Cidade Universitária, São Paulo, 05508-010, Brazil

[b] Nuclear and Energy Research Institute (IPEN-CNEN/SP), Center for Materials Science and Technology (CCTM), 2242 Prof. Lineu Prestes Av, São Paulo, 05508-000, Brazil

ARTICLE INFO

Article history:
Received 30 November 2016
Accepted 10 November 2017

Keywords:
Grain structure modeling
Interactive grain visualization
Physics-based simulation
Voronoi tessellation
Stereology
Grain boundary structure

ABSTRACT

This paper presents a novel approach that integrates geometric modeling and visual analysis of grain structures in an open source CAD system, aimed at educational purposes. An intuitive and simple automated modeling method produces valid polygonal representations of grain structures, by adopting a novel physics-based particle packing procedure with Voronoi-based tessellation. Models are structured to facilitate the development of interactive visualization prototypes in 3D interactive engines. Microstructural fidelity was pursued for the synthetic models to be accepted as representations of real materials. Meaningful sample's parameters such as mean number of neighbors and mean number of edges per face were replicated with acceptable precision, when compared to values obtained from 3D reconstruction of an alpha-iron sample. Domain-specific interactive experimental tools informed by learning and cognitive research sought to enhance spatial cognition of grain structures and support learning their fundamental features.

1. Introduction

The interdependence between materials' properties, processing and microstructure has been for long well known by scientists and engineers. The prediction of materials' properties that are more sensitive to microstructure is becoming an increasing necessity since novel applications require improved properties, demanding unequivocal and deeper understanding of such relationships. Recent research [1] discussed limitations of stereological methods typically used to assess grain properties, supporting the development and adoption of updated 3D characterization methods. Early experiments with 3D interactive visualization methods [2] allowed researchers to discover new features of cementite precipitates in high-carbon steel, asserting the limitations of 2D visualization and the potential of 3D interactive technologies.

Hornbogen [3], in a pioneering effort devoted to define the essence of microstructures, proposed the first comprehensive classification framework for microstructures based on geometric patterns. Recent work by DeHoff [4] demonstrates that the endeavor to clearly define and understand microstructures is far from finished, stating that microstructures are inherently 3D, space-filling, not-regular and not-random geometric entities and their description should be framed in terms of geometric concepts, reinforcing Hornbogen's stance. Therefore, it is paramount to invest in spatial exploration techniques that allow experiencing the inherent 3D geometric nature of microstructures and tackling complex visualization challenges such as the space-filling character.

Research [5,6] suggests that direct visualization and spatial interaction with phenomena of interest reduce abstractions, providing better support for understanding complex systems when compared to passive media such as text or images. It is known that spatial interaction aids deciphering complex systems by stimulating conceptual connections – cognitive maps emerge from detection of functional relationships and causal correlation [7]. Immersion and interactivity can also boost enthusiasm and attenuate learning barriers [5,6]. In this sense, adoption of interactive microstructural digital models can help unveiling grain size and shape, dislocation density, volumetric fraction, spatial distribution of phases and microcracks on a cognitive level. Engineering students are expected to benefit more from interactive models given that they usually have good spatial ability [5,7]. However, specific visualization mechanisms for learning purposes are still absent within materials research, especially in the microstructural scale

☆ This paper has been recommended for acceptance by A. Pasko.

* Corresponding author.
E-mail address: andre.montes.rodrigues@usp.br (A.M. Rodrigues).

https://doi.org/10.1016/j.cad.2017.11.001
0010-4485/

and valid and proper microstructural models are neither readily available nor straightforward to obtain.

A 3D object is usually represented by their boundaries (B-Rep) in most CAD applications. This type of data structure is also expected in powerful interactive development engines (or game engines) such as Unity, Unreal, Cryengine, Blender's game engine and also in web-based graphics libraries such as WebGL and X3D. Given this structure, interactive visualizations are simple to create with the resources available on such systems: rendering configurations for every object (colors, image textures and transparency), ready-to-use first or third-person controls, collision detection, object clicking and selection, raycasting and customizable user interfaces. Therefore, given the rationale of game engines, models of grain structures should be structured in a way that each grain is a single polyhedral object, allowing a high degree of control.

Traditional manual 3D modeling is unsuited to produce proper models and teachers are seldom qualified to create media content [8]. Dream 3D [9] and Neper [10] are relatively accessible tools capable of building microstructural models from user-defined parameters but are heavily research oriented, still lack integrated domain-specific visual analysis and interaction capabilities, the user interface is not friendly enough for educational use and the data structure of resultant models is not suited to use in 3D interactive software. Proprietary options such as Simpleware, Micress and Digimat suffer from the same issues and are not viable options as educational tools. Even if one knows how to operate such complex applications, the algorithms commonly used do not scale well to larger samples (more than 500 grains) or higher voxel resolutions, resulting in small models and poor visual quality. Therefore, simple, open source, automatic and integrated tools must be created in order to empower teachers, students, 3D content creators and even researchers, providing them with meaningful synthesis, visual analysis and interaction capabilities to allow advancement of teaching methodologies and comprehension of complex subjects such as grain structures. Models produced within 3D content creation CAD applications or game engines are easily captured and transformed by artists and ready to use within such applications or interchanged between them.

This paper indicates promising directions and contributes solutions for geometric modeling and interactive visual analysis of grain structures aimed at educational purposes, integrated in an open source CAD application. The goal is to support materials science classes for engineering courses. A novel and fast automated 3D modeling workflow produces polygonal valid 3D grain microstructures with data structures that facilitate the development of visualization prototypes in game engines. Domain-specific interactive experimental tools informed by learning and cognitive research are presented and the most prospective proposal was assessed in a preliminary user study. This paper is restricted to a grain model but the intention is to add other microstructural features (e.g. fibers, pores, second phases) and to investigate proper interaction techniques for those elements.

2. Modeling and visualization of digital grain structures

2.1. Digital reconstruction and modeling

In digital models the microstructural elements are usually simplified as a result of the construction method, e.g. stacking 2D images from serial-sectioned materials or simulating microstructure evolution [11]. The grain is the most relevant feature to be modeled, since it represents the fundamental segmentation of material space, defined by a phase shift or a change in crystallographic orientation. Therefore, microstructural models must represent a valid grain structure, from a statistical and a geometrical standpoint. The desired digital model is a hermetic aggregate of objects whose synthesis process is akin to other aggregates of interest in geological research, 3D content creation and gaming, such as piles of rocks or other objects, 2D textures and real-time object shattering [12–14].

Synthesis or reconstruction of microstructure models is usually performed in four stages [11]: Characterization, Synthesis, Geometric Extraction and Tessellation. The microstructural characterization stage is typically accomplished by application of stereological methods on 2D sections, advanced tomographic methods or grain-structure reconstructions based on serial sectioning [15–17]. The distribution data can also be arbitrary defined according to the application. Game engines and early materials models, for instance, used Voronoi tessellations constructed on a set of random points (Poisson distributed points) [18]. Some statistical descriptors of spatial arrangement of features in microstructures are functions (nearest neighbor distribution, radial distribution, K-function, two-point correlation and higher order correlation), tessellations (Delaunay, Voronoi, Dirichlet), Q-mode factor, surface to surface distance distributions, clustering and affinity parameters [19].

Synthesis stage relies on geometric methods or simulations that are specific to materials science (molecular dynamics, Phase Field, grain growth) to find one or more particle arrangements that exhibit requested microstructural features such as average grain size and grain size distribution. Further details will be given in the next section.

Geometric extraction stage aims building accurate grain boundaries from particle packing simulations or directly from statistical data, relying on algorithms such as marching cubes, marching tetrahedra and dual grid contouring or Voronoi algorithms. Finally, tessellation stage creates proper volumetric representations for finite element simulations, where Delaunay triangulations are acknowledged for producing high quality tetrahedra [20].

2.1.1. Geometric synthesis methods

Several solutions were proposed to tackle the synthesis stage in the creation of aggregates. Given the context of this research, geometric methods are more appropriate for they create simple but statistically valid instances of real samples, avoiding complex microstructure simulations. Numerous geometric methods have been developed, including random sequential adsorption (RSA) algorithm, Metropolis algorithm, Boolean schemes, Gaussian random fields, Gibbs process, Monte Carlo based techniques and the extensively used simulated annealing process [19]. Adequate reproduction of grain size distribution and topology must be enforced in the case of grain structures and geometric methods accomplish this by keeping the allowed overlap to a minimum in sphere or ellipsoid packing procedures. Optimum object packing has no trivial solution, particularly for free aspect ellipsoidal particles and success depends on initial conditions and particle mobility [21].

Simulated Annealing is a heuristic optimization method widely used for ellipsoid packing on microstructure synthesis procedures [11], where ellipsoids directly represent grain size and shape and the procedure tries to find one or more satisfactory packing conditions. Sampled ellipsoid particles are randomly distributed in space and then iteratively introduced, displaced or removed in order to simultaneously maximize packing and minimize overlap [11], a trial-and-error method that leverages no specific knowledge about the geometric nature of grain structures or ellipsoid particles. Homogeneity improvements are not guaranteed, for heuristics algorithms are approximation schemes and reproducibility is also challenging for they employ several random variables that must be recorded. In fact, Simulated Annealing is one out of many possible solutions to build space-filling aggregates from a known distribution, where any other iterative optimization algorithm can be applied. Literature also describes other similar

algorithms for this use, such as genetic algorithms [22] and the classic gradient descent solver [23].

On the other hand, physics-based packing simulations achieve packing by blending, vibration and compression. Optimization is achieved with abrupt shaking or by altering initial particle disposition [24]. This procedure shares the space-filling nature of grain structures and can take advantage of a comprehensive knowledge capital on mixing procedures, building on proven solutions to achieve better homogeneity and packing density. Despite the profusion of optimization algorithms such as Simulated Annealing, they are usually non-interactive inflexible black boxes designed to achieve fast solutions, not to be accessible to human reasoning. Ma et al. [25] is an interesting example of a 'mixed' method, combining both optimization and physics to obtain controlled aggregates of arbitrary objects. However, physics was only used to execute optional adjustments on eventual artifacts and their core solution is still an optimization scheme.

Physics-based simulations are inherently interactive, allowing one to experience the procedure in real-time, a feature that can be explored in educational settings. Simplified physics algorithms are accurate enough for visualization purposes and they are usually integrated in most 3D content CAD applications (Blender, Maya, 3D Max) and game engines (Unity, Unreal). The proposed method is reproducible and allows any degree of human intervention or creative contribution to the models, using any modeling and interaction tools available in the application, which is a valuable feature in this scenario. Finally, automated physics-based simulations allow easier result replication due to their deterministic nature. Therefore, since models for education are usually created in 3D CAD software by instructors, digital 3D artists and interaction programmers, the integration of physics engines is an empowering factor in this context.

2.1.2. Voronoi tessellation and grain topology

Voronoi diagrams subdivide space into convex polyhedral cells, shaping a hermetic structure (Fig. 2c). Voronoi tessellations are widely used on the tessellation stage of grain structure modeling due to simplicity and topologic similarity to metallic and ceramic materials, conforming to Euler's relation [26]. As attested by Underwood [16], average values approaches 15 for faces per grain and 5 for edges per face. From a metallurgical standpoint, traditional Voronoi tessellation can be considered the outcome of a homogeneous crystal growth process, whereas grain nuclei appear simultaneously, retain position along the process and grow isotropically until impingement [27].

2.2. Towards an interactive paradigm for visual analysis of grain structures

Lanzagorta et al. [2], in an early experiment with 3D visualization, were able to discover new features of cementite precipitates in high-carbon steel, demonstrating benefits of real-time interaction, interactive 3D and stereoscopic visualization, restating the limitations of static visualization approaches. This attempt revealed development opportunities and challenges on interactive visualization of microstructures, such as lack of integration of computational solutions and difficulties for end users to operate visualization systems and interact with models. In fact, it is the only initiative to date with clear intention to develop specific visualization tools for microstructures. However, the interaction aspects of this pioneering research were not further developed. Subsequent authors used visualization to satisfy specific research needs rather than developing specific interactive techniques for visual analysis of grain structures. On the other hand, this work has inspired development and adoption of digital grain reconstruction by serial sectioning, widespread nowadays.

It should be clear here what is meant by the term "visualization". According to Swan II [28], the most known aspect of visualization is rendering, where most fundamental problems were already solved. What this author considered as the greatest challenge of visualization is 'sensory design', involving human perception or cognitive processing, where the effort lies in representing abstract concepts, not realistic objects, in order to facilitate the understanding of complex phenomena. The goal is to define and emphasize the relevant features for a specific application while minimizing unimportant details and to establish a hierarchy of important relationships [28]. Accordingly, visualization is considered here as a domain-specific method that takes advantage of available filtering and rendering possibilities, orchestrated by an interaction rationale, in this case, aiming at novel interaction paradigms for grain structures.

The usual visualization approach of 3D reconstructed samples, as exemplified by Ullah et al. [29], is to use selective volumetric rendering, filtering features of interest such as grains and phases. Volume rendering specifies color and opacity levels for every voxel or 'volumetric pixel'. Static sections are obtained by surface rendering, extracting isosurfaces of the region of interest [30]. Beyond the possibility of satisfactory real-time rendering allowed by recent experimental libraries such as Gigavoxels [31], and information filtering capabilities, volume rendering is usually adopted within a static visualization paradigm that lacks domain-specific interaction techniques. There are several technical interaction requirements not satisfied by existing software and important materials' science concepts not adequately supported by such techniques.

Following Hornbogen's [3] and DeHoff's [4] formulations, microstructures have an inherent space-filling 3D nature and is paramount for a student to experience and capture geometric variations along a grain structure sample, which occur in regions where the grain size deviates from the average, concentrating large or small grains. Therefore, an elementary visual distinction between big and small and, especially, bigger and smaller along a given sample, seems an important prerequisite for proper analysis and detection of heterogeneous regions. The next step in this formulation of a grain structure visual analytics is to detect punctual (or neighborhood) and local grain size concentrations. Other relevant concerns for educational applications are offering user-friendly interfaces, as indicated by Lanzagorta et al. [2] and exploring visual design and aesthetics to improve cognitive performance in visualization experiences [28]. Exciting interactions can also contribute to boost user engagement [6].

2.2.1. Interactive visualization possibilities

Real grain structures are traditionally visualized with 2D sections, aiming characterizing grain properties by way of stereological methods [16], which is being questioned for visualization purposes and also for materials characterization [1]. A clear limitation of single sections is that it cannot reveal much about the geometry of the sectioned grains or spatial relationships. In fact the exclusive use of sections usually leads to misconceptions about grain shape and size among students. Interactive sectioning can help eliminate such misconceptions [2], allowing infinite sections to be visualized continuously in a brief period, an ideal solution on a cognitive visualization perspective. The original video sequencing technique introduced by Lanzagorta et al. [2] was not further investigated in the literature. Interactive sectioning in first person pushes this idea further, allowing more freedom and a larger sample to explore. However, in a first analysis, sections are computationally intensive procedures executed by surface rendering methods for volumetric models and Boolean operations for B-Rep models, limiting interactivity. This is the reason why most software execute sections in discrete steps. The software Graphite [32] is an interesting example that allows the user to interactively select

the section plane angle, although the feature is limited to rotation around a central pivot.

Multiscale visualization is a promising interactive approach for learning purposes because it aims representing models as close as we experience in reality—real objects show more details as we approach them. The term encompasses methods to deal with models that have details on several spatial or even temporal scales, exceeding eye resolution [33]. However, multiscale models challenge traditional 3D modeling and visualization paradigms, since the quantity of objects can scale to billions. In this sense, for some applications the only viable approach to modeling is automation with procedural [34] or tiling techniques [35] or to avoid modeling at all by adopting alternative or statistic representation of groups of objects.

In the case of grain structures two scales are of particular interest, the grain scale and the atomic scale. An automated process to model valid synthetic grain structures is presented in this paper, with a proper data structure for multiscale visualization in interactive engines. Modeling of atoms in a given crystal structure, including atomic defects, can be done procedurally, as geometric rules of such structures are known and clear. Conventional visualization would demand huge amounts of storage and graphics capacity. The solution is to balance quantity and quality, controlling the computational load, based on the premise that is senseless to display more objects than we can perceive, offering an automatic and intuitive filtering rationale. Common techniques are frustum culling (limiting what is visible), LOD (varying level of detail of objects) and scene partitioning schemes (on-demand loading of scene sectors) [33], commonly available in modern game engines.

Visualization in multiscale environments also poses cognitive challenges. Typical issues are navigation on crowded and occluded environments, localization within a large world, acknowledgment of data in other scales and scale transitions. Solutions are assisted navigation, filtering and zooming, secondary windows, contextual maps or hierarchical trees, alternative representations of objects with icons, as well as symbols and hyperlinks. Such solutions are easily implemented in game engines.

The authors hypothesize that an orchestrated combination of the methods discussed so far can deal with the space filling character of grain structures and simultaneously allow inspecting characteristics of single entities, detecting heterogeneities, analyzing local relationships and distributions. The first goal is to offer an improved learning experience over traditional educational media (such as images, diagrams an animations) or available visualization software in order to tackle typical student misconceptions. Prototypes are described and presented in next sections.

3. Materials and methods

3.1. Software

Ghosh et al. [36] used a CAD system to build more accurate representations of grains, automating the modeling workflow using the application programming interface. This work inspired the strategy to design an integrated and automated workflow comprising 3D modeling and visualization in an open source CAD suite, leveraging built-in tools and interactive technologies. Most contemporary 3D content creation CAD systems integrate animation tools, physics engines, scripting capabilities and even game engines, creating an ideal environment to build specific interactive visual analysis tools for grain structures.

The ideal application should be lightweight, free, open source, easily customizable, equipped with powerful modeling and computational geometry features and have wide support from the user community. From several options available, Blender 3D [37] satisfied all requirements. A relevant feature is that almost all built-in tools and functions are accessible through a friendly Python API, easing workflow automation, customization and creation of new tools.

3.2. Geometric modeling automation

Automation challenges and data requirements were assessed by a manual workflow, obtaining proper rules to create automated scripts for eight identified steps:

- Grain size distribution data
- Grain size sampling
- Particle list
- Particle representation
- Particle modeling
- Random particle placement
- Particle packing
- Grain modeling from final particle positions.

As expected, the last two steps were the most challenging. Considering that models should have more than 400 grains, from a practical visualization perspective, almost all steps needed to be automated given the workload to create and position all grains.

3.3. Particle packing and tessellation procedures

A simple and intuitive particle packing procedure based on physics-based simulation was favored over simulated annealing due to implementation and operation simplicity and wide availability of good engines and algorithms embedded in modeling applications. Blender integrates the awarded Bullet Physics library, offering several settings and customization of physical behavior of objects. Avoiding the need for powerful workstations, the particle representation should be light in terms of triangles but geometrically accurate enough for the packing procedure. Icosahedron was found to be a good substitute for spherical particles (see Fig. 2b) and is conveniently available as a procedural object on Blender. Currently, the collision object type was set to a sphere primitive, as grain shape is not considered in this work and due to faster collision calculations.

The approach was inspired by blending methods, therefore early designs adopted gravity and shaking (Fig. 1). However, this strategy created undesired heterogeneities in distribution. The final packer was chosen due to superior particle packing and minimal grain size concentration gradients in the resulting grain model (Fig. 1c), composed of six movable walls and running on a gravity free environment. A high damping factor was imposed on the movement of particles, ensuring that movement is exclusively caused by wall displacement, avoiding the accumulation of smaller particles in between the interspaces. Particle position is randomly set to one spot of a configurable grid, until all positions are filled (Fig. 2a).

The procedure approximates particles gradually to the contact, finishing when the particle assembly reaches specified levels of vibration (video 1). This procedure was firstly executed by manual control of two groups of platforms, reducing the height (top and bottom platforms) and width (4 lateral platforms). Platform movement was coordinated to achieve the desired compression (vibration), homogeneity and shape (square sample).

Video 1. Packing procedure (Appendix A).

3.3.1. Packing control algorithm

A script was created to control and coordinate the movement of the six platforms:

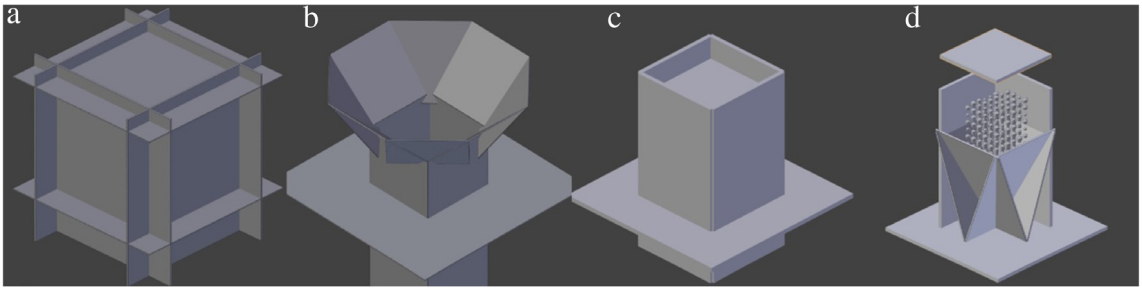

Fig. 1. Particle packers.

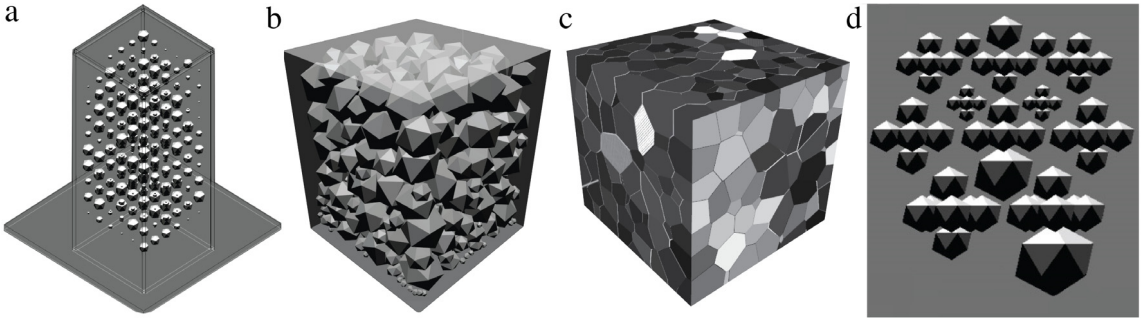

Fig. 2. Geometric modeling procedure. (a) Random particle arrangement in the virtual packing device. (b) Packed assembly. Each particle is represented by icosahedron (regular platonic solid with 20 triangular sides). (c) 3D Voronoi tessellation. (d) Particle clusters designed for grain size adjustments.

- 8 innermost particles are identified;
- Simulation speed is set to slow;
- Simulation is started and each group of platforms moves at constant speed;
- Given the predefined speed and 30 s total simulation time, the vibration level measurement was defined to start at 20 s;
- Vibration levels of 8 innermost particles are measured every 5 simulation frames (6 times per second) by calculating particle speed.
    - Levels are checked against experimentally set limits—too much vibration indicates interpenetration. This stoppage condition guarantees enough compression along the sample volume.

It should be noted that parameters can be modified to obtain different results. If sample geometry is changed, for instance, one can create one-grain-thick films and rods while dumping, gravity and force parameters allow introducing controllable heterogeneities that can be applied to model functionally graded materials.

The simulation produces a packed particle assembly (Fig. 2b) and one planar-faced convex polyhedron is created for each particle by the Voronoi algorithm (Fig. 2c), placing a perpendicular plane at the medium point of each line segment between two neighboring particle centers (Fig. 3a). Blender's Voronoi algorithm was modified to increase performance, to include relevant measurements and for integration in the automated workflow. Implementing the Voronoi algorithm as a Python script compromises performance but assures high compatibility, as it runs in most Blender versions in all supported operational systems. Every generated face is duplicated and assigned to a Blender object, allowing controlling graphical properties of each grain and easy measurement of geometric properties.

Resulting models can be exported to several typical 3D file formats such as STL, OBJ, FBX, PLY, DAE and X3D, allowing the use of other 3D graphics applications or interactive game engines and also 3D printing tools.

3.4. Topology, grain size measurement and distribution curve control

Models ranging from 350 to 1050 grains were validated by microstructural topological parameters, namely average values for faces per grain and edges per face, historically adopted to describe geometric properties of grain structures [3]. Since new definitions are being formulated by the scientific community, those parameters were adopted for comparison purposes.

An assessment of parameters sensibility to the size distribution of particles was executed. Test batteries adopted 1, 2, 3 and 7 particle size classes and amplitudes randomly chosen within log-normal curve limits (from 20% to 260% of the average size). Class frequency was constant or uniform. Finally, each battery contained five samples, with a randomly defined particle size for every class (see Table 1).

The final size distribution was kept close to the log-normal pattern, regarded typical of polycrystalline materials [16,17,38], based on a specific Iron grain size distribution directly measured in 3D from a virtual model obtained through serial sectioning of a real sample [39]. From this data and the desired number of grains, a list of particle radius was generated, one for each grain. The normalized distribution was then measured and compared with the reference by way of a modified chi-squared test [17].

Grain size is traditionally estimated from 2D sections and not measured in 3D. In our case grain size was expressed as the diameter of the equivalent volume sphere, as described by Exner [17]. The Iron reference [39] also used this method (radius instead of diameter), which allowed a direct comparison of topology parameters. Grain volume can be precisely obtained in the generated model, using a known tetrahedron volume calculation procedure, usually available as part of math libraries in most 3D software and game engines. This procedure requires that each polyhedron grain is divided into several tetrahedrons. By using the center of the grain as a common vertex it is possible to complete a tetrahedron for every triangular component, given that each planar face in Blender is formed by several triangles.

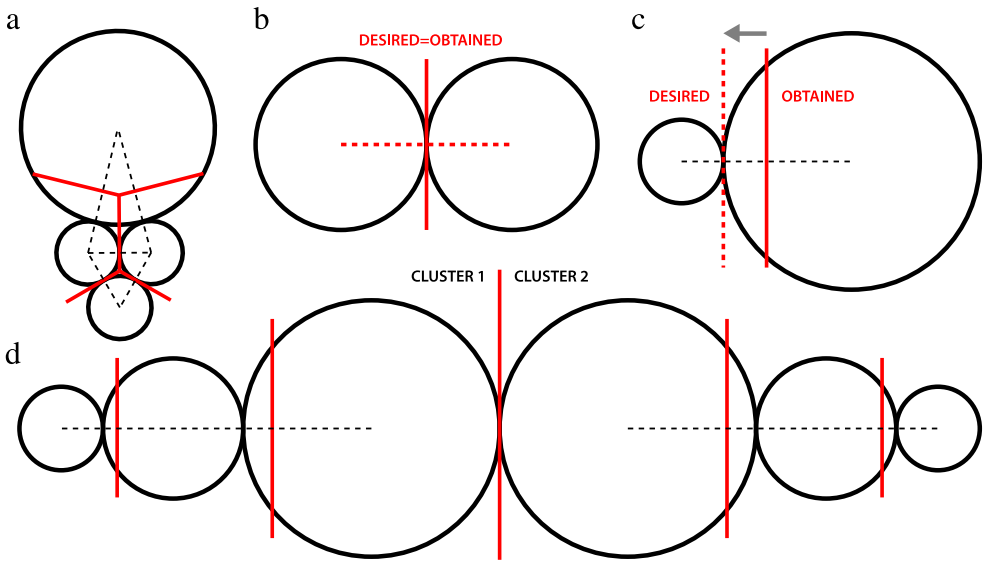

Fig. 3. Grain size disparity: (a) Voronoi diagram construction; (b) Equal particle sizes—plane is accurately positioned; (c) As the size difference increases, the plane deviates from the desired position; (d) The adoption of a particle size gradient reduces the average of discrepancy in plane position.

Table 1
Grain topology parameters.

			Number of particle size classes				Overall average	Ref. [29]
			1	2	3	7		
Faces per grain (average)	SAMPLES	1	12.6	12.8	12.0	11.7		
		2	12.7	12.3	12.0	12.0		
		3	12.6	12.1	12.1	11.7		
		4	12.7	12.2	12.0	11.9		
		5	12.6	12.3	12.1	12.2		
		Avg.	12.6	12.3	12.1	11.9	12.2	12.8
Edges per face (average)	SAMPLES	1	4.8	4.8	4.8	4.9		
		2	4.7	4.7	4.8	4.8		
		3	4.8	4.8	4.8	4.7		
		4	4.7	4.8	4.8	4.9		
		5	4.7	4.8	4.8	4.9		
		Avg.	4.8	4.8	4.8	4.8	4.8	4.9

3.5. Visualization

The goal of this research in the visualization realm is to obtain instructive interaction methods for complex microstructures, comprising all typical phases and defects. However, since grain structure is considered the most fundamental feature of microstructures and no specific interaction method exists yet, this paper shows experimental methods to interact specifically with grains. Prototypes were developed and preliminarily evaluated with support from teachers and students, progressing from simple interactive visualizations that anyone can perform using existing Blender's functionalities to a domain-specific experimental tool (interactive sectioning) and other promising possibilities allowed by combinations of both.

3.5.1. Basic interactive mode

The procedure aims tackling relevant visualization challenges such as occlusion by creatively exploring and combining Blender's available features. Simple scripts were created to automate batch modifications on objects, such as changing materials settings and applying geometry modifiers. Built-in first-person navigation methods were used, where the 3D view is positioned at eye level, enabling one to move around the 3D scene as if "flying" through the model.

3.5.2. Dynamic section mode

Instead of executing computationally intensive Boolean operations between the section plane and sectioned objects, a simple technique was conceived to obtain sections in real time, allowing first-person interactive fly navigation. The camera's near plane was set as the section plane. Backface culling was disabled so the interior side is visible and then rendering was configured to discard the shade component so all faces reflected the pure RGB color of the grain, creating the illusion of a solid section. Another version was created without this feature, allowing the user to see the remaining grain portion behind the cutting plane. In order to visually distinguish the section plane from the rest of the sample a transparent yellow casing was created.

A complete setup was created to allow an easy and full experience with the tool, based on best practices for interactive systems. A 'world map' window aids users locating themselves inside the sample. A Python script handles some interface configurations such as initial camera position and direction and builds a graphic interface, including buttons to start and stop the interaction, reset the camera to the initial state and take screenshots.

3.5.3. Multiscale mode

This prototype was created to assess computational and cognitive issues of multiscale visualization. Once again a Python script was created to automate interface configurations. The user navigates in first-person fly mode. Again, a secondary 'world map' viewport was created to aid users locating themselves inside the sample.

The essence of the multiscale algorithm is that grain visual representation changes according to its size on screen. This parameter should be set to properly show the detail level that is actually visible at that scale. In order to avoid unnecessary computational overhead, the algorithm runs at every 5 frames (12 times per second) only on visible objects. This update rate was found to be satisfactory for real time interaction, given a predefined appropriate navigation speed. The algorithm is detailed below:

- Bounding box and distance from camera are obtained for every visible object;
- User clicks, target and relative screen sizes of grains are obtained from internal events variables;
- Values are checked for five conditions:
    - Click detected: only the clicked object is set visible for individual inspection.
    - Very small size on screen: the grain is too far away and little detail is visible. Grain representation is set to a lightweight 3D icon so the system is able to represent numerous groups of grains;
    - Small size on screen: grain is big enough so geometric details can be seen. Representation is set to standard (opaque color);
    - Medium size on screen: surface details can be revealed. In this exploratory stage an image texture was used to represent a random crystallographic orientation. The intention is to show features of the next visible scale, the crystal lattice in this case;
    - Large size on screen: the grain occludes the view. Object's alpha channel value is set low and the grain turns transparent allowing the user to wander inside the sample. The intention is to show features of the next visible scale, groups of atoms in this case.

4. Results

4.1. Topology evaluation

The synthetic samples precisely reproduced the topologic parameters defined by the references, for values obtained either by stereology or directly in 3D, related to metallic materials (Table 1). For the grain size distribution, direct three dimensional alpha iron data was used as reference, according to Ullah et al. [29] and Zhang et al. [39]. Average face count ranges from 11.9 to 12.6 (reference values are 12.15 [39] and 12.8 [29]). Average values for edges per face were 4.8 (reference value is 4.9 [29]). The values excel random distributions of Voronoi seeds and Kelvin's tetrakaidecahedron, especially in face count results (15.5 and 14, respectively [27]). It should be noted here that Kelvin's tetrakaidecahedron was deemed for a long time the best representative shape of an energetically balanced grain.

4.2. Grain size distribution

Exploratory models using one or two particle sizes resulted, respectively, in unimodal and bimodal distribution curves, as expected. However, grains from bimodal samples already displayed slight size deviations when compared to their particles. This deviation was amplified when different particle sizes were introduced. In fact, as already reported in the literature [26], the Voronoi diagram causes a discrepancy in size between the source particle and the generated grain, for the boundary plane is always positioned halfway the neighboring particles regardless of particle size (Fig. 3a). This causes a decrease or underestimation of larger grains and an increase or overestimation of smaller ones, narrowing the distribution curve. Still, it should be emphasized that the variation of the particle distribution curve introduced in the simulation had little influence on the analyzed geometric parameters.

In a second phase, an artifice was devised in the particle sampling procedure to dampen the effects of the traditional Voronoi diagram, using specific particle clusters in order to get closer to the desired distribution, yielding some interesting results. Although weighted versions of the Voronoi diagram can tackle this issue [40], this option was pursued in order to preserve the simplicity of the original Voronoi algorithm and to investigate alternative modeling solutions. A cluster is defined here as a set of particles which can be either in full contact or slightly spaced apart, assuring that the established neighboring between particles will be maintained after the compression. The creation of such clusters observed the following hypothesis: a grain will have its size similar to its generating particle if accompanied by other particles of similar size to the end of compression. Fig. 3 illustrates this concept, showing that the boundary plane is exactly positioned at the interface point between neighboring particles of the same size (Fig. 3b), but is moved away from the contact point as the size difference increases (Fig. 3c).

In other words, the smaller the size difference of neighboring particles, the more accurate the position of the boundary plane. Therefore, arranging the particles of a cluster observing a size gradient (Fig. 3d) results in less distorted grains. On the other hand, when pushing this concept to the extreme, undesirable heterogeneities would be created either through accumulation of grains with the same size or the establishment of artificial gradients. Thus, particle clusters were created (examples in Fig. 2d) with few particles of the same size, in an iterative process aimed at adjusting the distribution curve, particularly at its tails. Then, the packing process was executed again with the particle clusters instead of previous isolated particles (video 2).

Video 2. Packing procedure with particle clusters (Appendix A).

The outcome of this process was deemed satisfactory, increasing the distribution curve amplitude and approximating its values to the reference (Fig. 4). The chi-squared (X^2) was 6.7, which, according to Exner's interpretation [17], results in a probability of coincidence of distributions of approximately 90%.

4.3. Computational performance of simulation and tessellation procedures

As expected, the most demanding procedures were particle packing and Voronoi Tesselation. The impact on performance and execution time of the other procedures can be considered negligible. For microstructural models up to 1050 grains in the target hardware (dual core processor laptop, 2 GHz, 4 Gb RAM, integrated GPU), particle packing alone consumed around 30 s at 30 frames per second (or 900 physics iterations), given that the built-in physics engine runs in real time, i.e., the packing procedure has a speed akin to reality and 30 s was found to be enough for proper packing and stabilization of particles. This type of simulation scales quadratically with the number of particles, however, whenever big samples are necessary, it is possible to pack particles in batches, where previous batches contribute only the resulting boundaries. In this strategy, not implemented yet, the packing procedure may

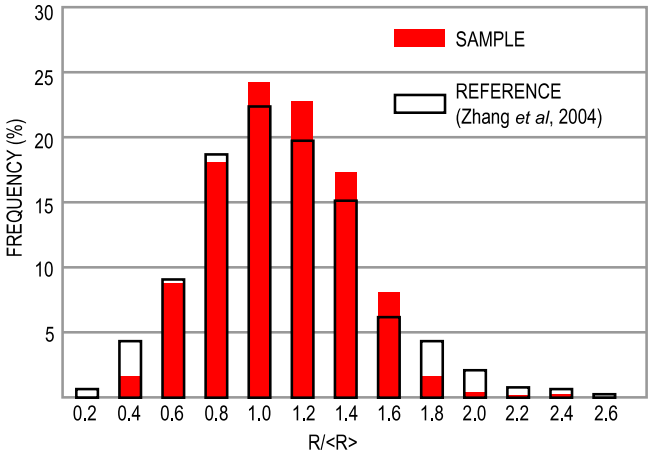

Fig. 4. Distribution comparison (sample versus reference). Grain size was measured by equivalent spherical diameter method. Radius (R) was normalized by average value ($\langle R \rangle$)

scale linearly with the number of particles, a clear advantage over conventional simulated annealing, for instance. Other possibility is exposed in [35], where especially designed interchangeable pieces called Wang tiles can be combined to obtain samples of any size, maintaining structural characteristics. Despite the possibility of greater time savings, the method would still have to deal with interfacing, i.e., how to obtain the tiles.

The Voronoi script takes approximately 10 s to create 1000 polyhedral grains. However, in this algorithm execution time is linearly proportional to grain count, as the average number of contiguous particles is constant and unrelated to sample size. Therefore, this algorithm can be used as it is for any sample size. It must be noted that the custom code runs on Blender's Python API, that is optimized for native operation calls, not heavy calculations, meaning that the execution time can be further reduced if necessary. Although not optimal, as stated before, this scripted implementation in Blender is more compatible, accessible and configurable. Whenever performance becomes an issue and when integration, compatibility and ease of use are not relevant concerns, optimized external applications such as Voro++ [41] can be used instead. However, 10 s was considered fast enough for this procedure and further optimizations are not needed for small samples and educational purposes.

Overall, samples up to 1050 digital grains were produced in less than a minute.

4.4. Interactive visualization prototypes

4.4.1. Basic interactive mode

Fig. 5 shows possibilities of Blender's standard built-in mechanisms. Examples (Fig. 5a) reveal challenges to comprehend grain shape, size and spatial structure, due to heavy occlusion in space-filling solid structures. Options to deal with occlusion are transparency (Fig. 5b, j), wireframe rendering (Fig. 5e) and selective masking of objects (Fig. 5c–l). Orbital navigation is (centered at the selected object) and first-person fly navigation aid in revealing the 3D structure through movement. Single image rendering or nearly real-time interactions often result in superior image quality but limit interaction (Fig. 5h, i, k, l). However, such options allow one to improve volumetric perception or highlight features of interest such as grain edges (Fig. 5l). The possibility to alternate from simple real-time first-person navigation to high quality static representations allows balancing volume (quantity of objects) and detail.

The best technique to explore the grain model found in this scenario was to experiment with real-time rendering modes (Fig. 5a–g), alternating from opaque to transparent representations, navigating around selected grains or dwelling in first-person mode (Fig. 5e–j) while showing and hiding grains manually (Fig. 5c–l). Free exploration with rotations and fly navigations allows the user to capture size and shape of single grains, to verify immediate neighbors (Fig. 5e) and to have a grasp on the 3D topology.

Despite no formal experiment was realized, it is clear that the cognitive performance of basic visualization techniques depends on user's spatial abilities, exploration time and, most importantly, good software knowledge. Since engineering students are expected to have good spatial abilities [5,7], the proposed methods should perform well for the target audience. However, learning complex software is not feasible in educational contexts.

4.4.2. GrainCrawler tool

Given the surprising results of basic techniques, the best combinations were further studied in an experiment, resulting in the GrainCrawler (GC) tool (video 3). GC allows the user to seamlessly navigate in first-person through the sample, focusing on exploration on a grain-by-grain basis, assessing size, shape and how many neighbors a grain have but still able to capture structural information (Fig. 6). To achieve this several procedures, features and tools explored in the basic mode were combined. The radius effect of a point light helps distinguishing nearby grains and evaluating grain density in the region (Fig. 6a, d). Auxiliary wireframe cages allow easy recognition of faces and number of neighbors and the transparent faces allow one to see geometric characteristics of all nearby grains (Fig. 6b, d, e).

Video 3. GrainCrawler Tool (Appendix A).

4.4.3. Dynamic section mode

Fig. 7 shows screenshots of the dynamic real-time section prototype (video 4). The interaction allows the user to visualize 'infinite' sections from the sample, on any angle, using first person navigation. A preliminary user study was performed to check if users are able to detect relevant geometric heterogeneities along the sample (specified in Section 2.2). Four tasks were designed: detecting 5 bigger grains (Task 1 or T1), 5 smaller grains (T2), inspecting the shape or aspect ratio of a single grain (T3) and detecting two big grain clusters and two small grain clusters (T4). Fifteen participants from the target audience (engineering, chemistry, physics and biology) were selected among research staff members not directly involved with this project. This group took part of a one hour exercise, applied in a computer laboratory using standard desktop computers. Days before the exercise, participants answered 10 questions about their background in 3D graphics applications, drawing and relevant personal traits (persistence, patience). The questions aimed to indicate previous experience or training in the navigation technique, spatial ability level and any positive or negative factor (stimulus, impatience) that may impact the results. A five minute navigation tutorial was held to avoid learning interferences in test results. Performance (correct answers) and task time were measured objectively and a follow up questionnaire was applied to assess mental stress levels and stimulus or joy using the system. Task order was counterbalanced with a balanced latin square scheme to avoid order effects. Such factors are usually assessed in user studies, as they usually correlate with performance results and might explain unexpected values or behavior.

Time and scores response distributions as well as their residuals were found normal according to Shapiro–Wilk tests, conforming to ANOVA normality assumption. Only T1 ($p = 0.0076$) and

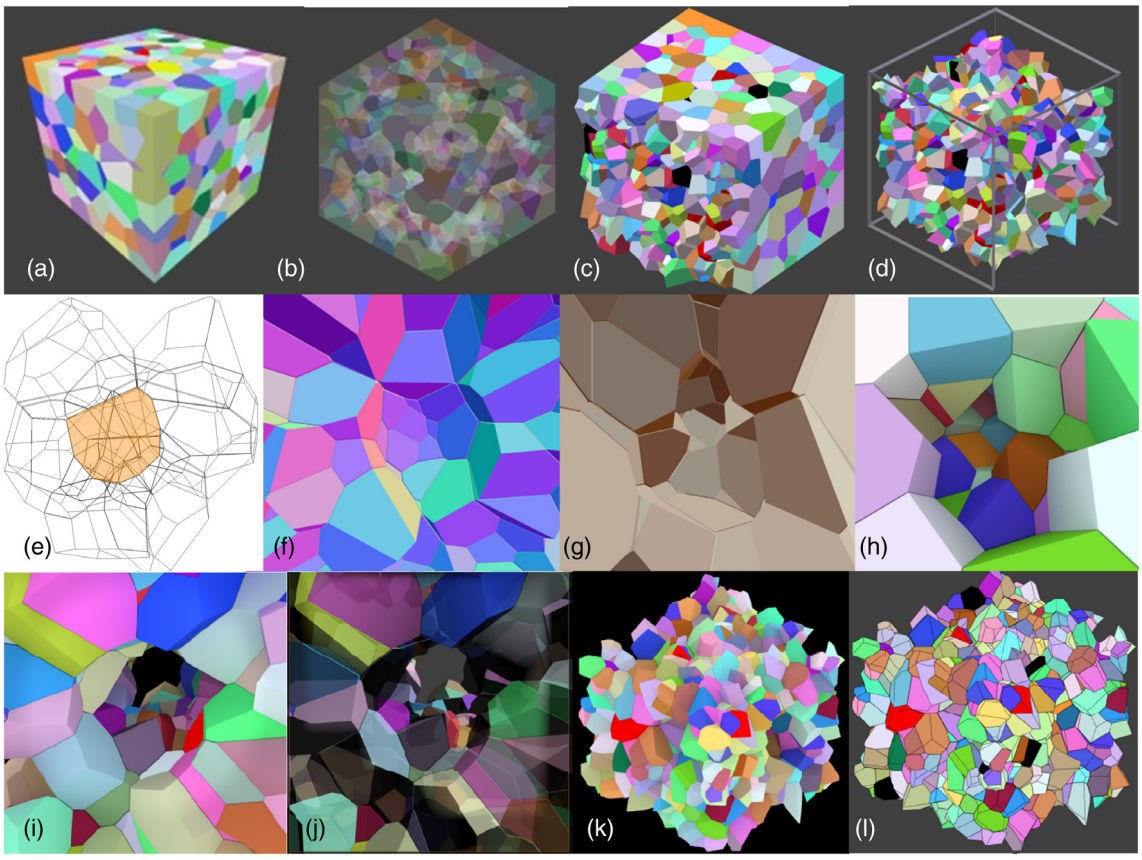

Fig. 5. Basic visualization mode. Real-time techniques: (a) perspective rendering. (b) Transparency. (c, d) Manual removal of boundary grains. (e) Close examination of 14 neighbors of a specific grain in wireframe mode. (f, g) Manual removal of grains, different rendering methods. Nearly real-time: photorealistic rendering with (h, i, k) manual removal, (j) transparency and (l) edge rendering.

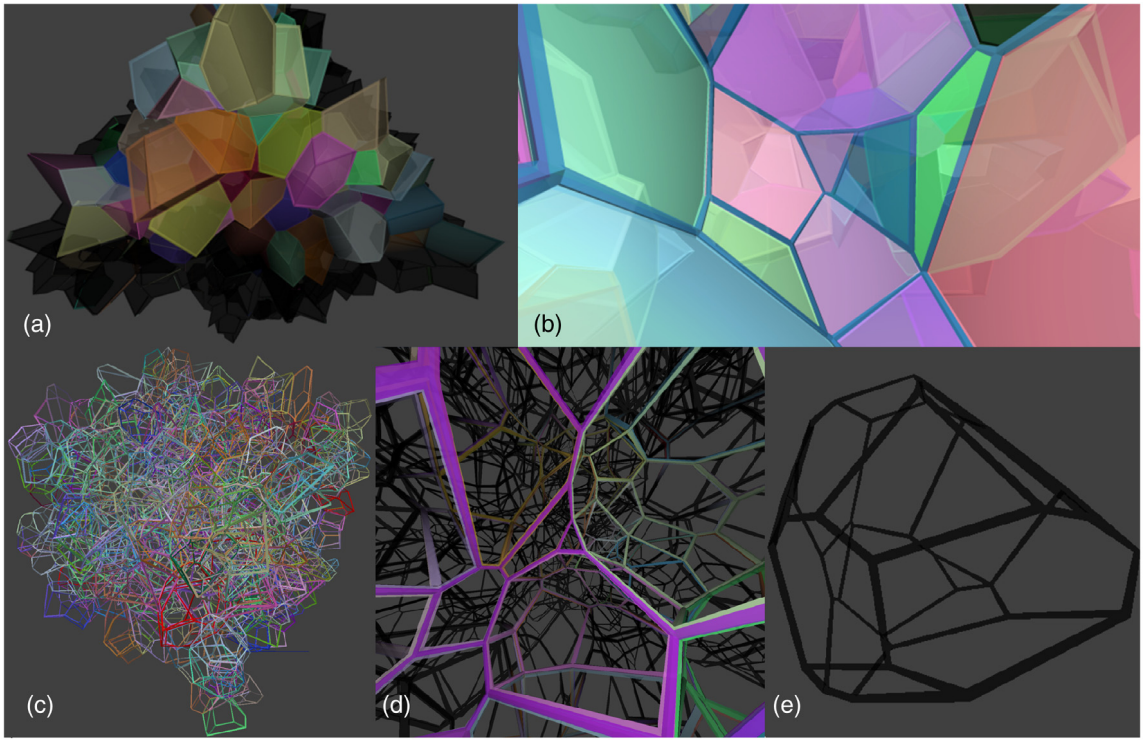

Fig. 6. GrainCrawler Tool. (a) Approaching the sample. The radius effect of the point light can be perceived. (b) Inside a big grain. (c) Alternative version with faces removed, (d) evaluating grain density in the region. (e) Grain isolation.

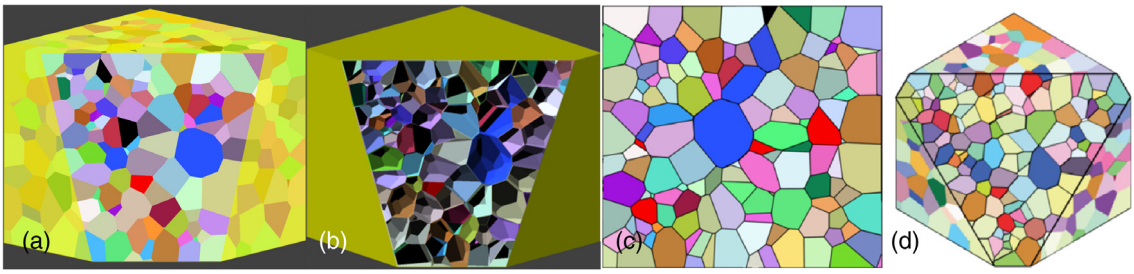

Fig. 7. Dynamic section mode. Images are extracted from the interactive tool. (a) Flat 2D rendering of plane section. (b) 3D rendering of plane section. (c, d) Screenshots (not real-time) enhanced with stroke rendering.

T4 ($p = 0.035$) scores deviated from normal although T1 was probably normal for their residuals did not deviate significantly from normal. T4 was further tested and passed the Kolmogorov–Smirnov log-normality test. T1 and T2 tasks had similar rationales (search for grains by size) although participants performed better in T1 (T1: 4 out of 5; T2: 2/5), probably due to the fact that bigger grains are easier to detect, a hypothesis reinforced by longer T2 average task time (T1: 234 s; T2: 375 s). All participants were able to guess a close grain shape in T3, considering that the definition of shape was somewhat vague. Since grain heterogeneity is not a common terminology or easily recognized property, surprisingly all participants were able to find at least two correct 'epicenters' in T4 (most found 3 out of the requested four), as defined by experienced evaluators that have explored the sample for a long time.

Despite some clear advantages over previous techniques, the view is always 2D. Fig. 7b demonstrates a variation of this technique that reveals the remaining geometry of the sectioned grains. A stereoscopic version can be used on a 3D monitor, giving the user superior depth perception and a full 3D experience. It is suggested that the 3D enhanced versions will shorten substantially the time needed to capture grain geometric characteristics even in a given static position. Finally, a screenshot tool allows extraction of static sections with enhanced border lines, obtained with Blender's Freestyle rendering functionality (Fig. 7c, d), allowing creating visually appealing sections or even animations.

Video 4. Dynamic section prototype (Appendix A).

4.4.4. Merging techniques, alternating and combining representations

Fig. 8a–d shows relevant examples of combination possibilities of techniques shown before, where grain size and shape can be better appreciated in 2D visualization by way of depth perception enhancements (Fig. 8a) and filtering allows close inspection of specific grain groups and neighbors (Fig. 8b–d). An experimental voxel representation (stair-stepped boundaries, see Fig. 8e–g) allows visualizing crystallographic orientation and the misorientation at the boundaries (difference in crystallographic orientation between two grains). This feature also adds dynamism and more realism to grain boundaries.

Fig. 9 shows the visualization possibilities of alternating and combining some or all the representation modes (video 5) aiming, in this example, to highlight grains, boundaries and neighboring relationships. One can see that various combinations are possible.

Video 5. Alternating techniques (Appendix A).

4.4.5. Multiscale mode

Fig. 10 shows screenshots of the experiment on multiscale interaction (video 6). The algorithm balanced volume and detail maintaining graphics load within proper range at all times. This means that the introduction of more grains is less likely to impact performance. Visual performance was addressed by means of preliminary experiments. It is clear that some visual transitions are not natural for all users but after a brief training period their purpose becomes clear and the benefits arise. The automatic transparency and grain picking features allowed instant appreciation of grain size, shape and neighbors.

Video 6. Multiscale interactive prototype (Appendix A).

As expected, no performance issues were found either on standard visualizations or the dynamic section tool, since no special computations are necessary. On the other hand, as verified in the preliminary experiment, multiscale visualization poses several challenges for real time applications. Despite that the actual system has only one scale, the main computational challenges were assessed and a real time visualization of more than 1000 grains were achieved, running always over 30 frames per second on conventional laptops (dual core processor, 2 GHz, 4 Gb RAM, integrated GPU). The same algorithm can be applied to change representation modes of objects in other scales given that total scene objects are kept within limits. Such limits were not established, since they depend on object characteristics. Additionally, a scene partitioning scheme to control the quantity of objects in the scene was not implemented yet.

5. Discussion

5.1. Geometric modeling

Features were chosen in pursuit of a fast, effective and flexible geometric modeling method to obtain properly structured polygonal models for use in game engines and not to compete with simulations, that try to reproduce physical and chemical phenomena that occur in the formation of real materials. However, simulated annealing can also be considered a geometric modeling approach and, in this sense, physical packing can be further developed to produce better results in terms of packing. In short, the packing procedure is still not a competitor in the digital materials synthesis arena, but it does a great and fast job to obtain visualization ready samples of considerable size. The comparison between the methods is an interesting research topic for future work.

This is the first work to our knowledge to adopt physics-based packing for grain modeling and, most importantly, to achieve positive results. Our method allowed a valid 1000 grain structure to be built in less than one minute, already in a lightweight structured polygonal form, ready to use in game engines. For bigger samples, as already discussed, physical packing can be adapted to be executed in stages, achieving close to linear execution time. In Dream 3D [9], for instance, execution time does not scale linearly as grain count or resolution increases. In fact, only small and low resolution grain structures can be built within 1 minute and the resulting model is 'voxelized', demanding additional processing time to create smooth and watertight geometry, besides special

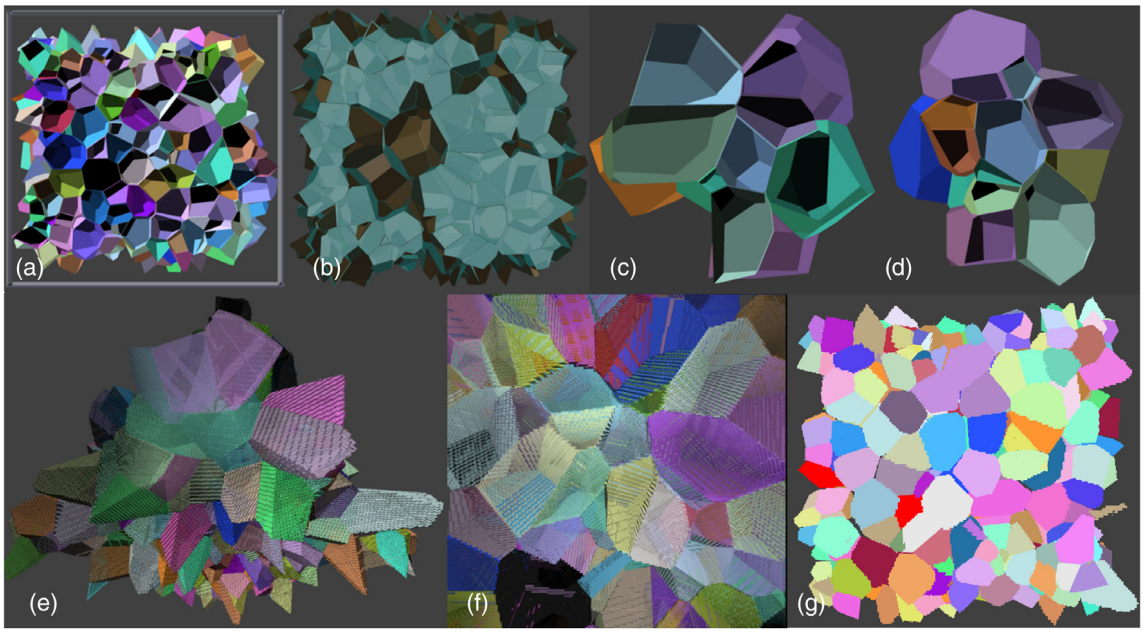

Fig. 8. Combined techniques. (a) '3D' sections with filtering (selective removal of grains). (b) Filtering and shading to highlight sectioned areas. (c, d) Isolation (14 neighbors of a given grain) and section. Stair stepped boundary models (e) allow communicating crystallographic orientation: (f) transparency and (g) flat shading in dynamic sectioning.

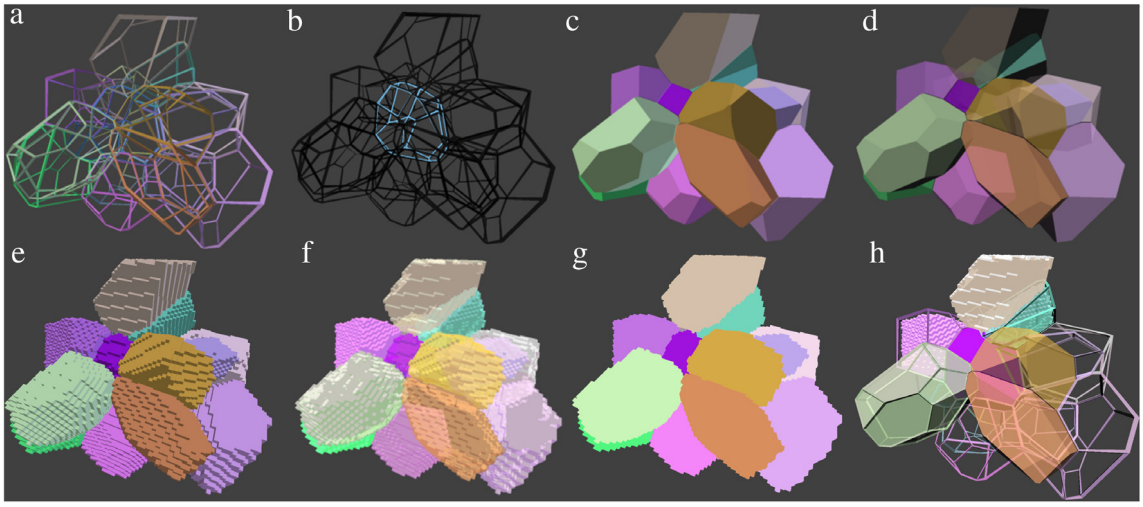

Fig. 9. Alternating techniques to visualize grain neighbors. (a) Wireframe cages. (b) Highlighting grain of interest. (c) Opaque and (d) transparent solid. (e) Opaque, (f) transparent and (g) flat shaded stair-stepped solid. (h) Merging representations.

procedures to convert such models to the form expected in game engines.

Real time packing procedures are relevant in several fields, for simulation and dynamic visualization purposes. In this work one has seen only static grain structures, but the inherent interactive character of physical particle packing not only allows easier human intervention in the process but can also be used to illustrate, in an educational context, dynamic processes that occur on formation and transformation of grain structures and even material processing methods such as powder metallurgy. Blender has also soft tissue simulation capabilities that can be applied in this scenario. Such dynamic illustrations are to be explored in further developments of this work.

On the tessellation side, the legitimacy of Voronoi-based virtual microstructures has been questioned in several studies. Two limitations arise when a grain is represented by a single Voronoi cell. Firstly, although grains may have concave regions, Voronoi diagrams are limited to produce one convex cell per reference point. However, this simplification is commonly accepted by studies due to time savings, especially for bigger samples, and is completely acceptable for educational visualization purposes. It should also be noted that only simulation approaches can produce natural grain surfaces and such methods do not use tessellation at all.

The second limitation of the Voronoi diagram, confirmed in this work, is size disparity between simulated particles and resulting grains. Voronoi diagrams built on randomly defined seeds result in overestimated face counts per grain, underestimating grain size distributions [26]. This issue could undermine the value of the packing procedure for the synthesis process. However, grain topology has proved to be independent from particle size distribution and the good agreement to referenced values derived directly from the simulated packed particle assembly, yielding the samples to be valid microstructural models that possess relevant features of real materials.

The novel particle cluster artifice significantly restored the original particle sizes. However, grain distribution comparison failed

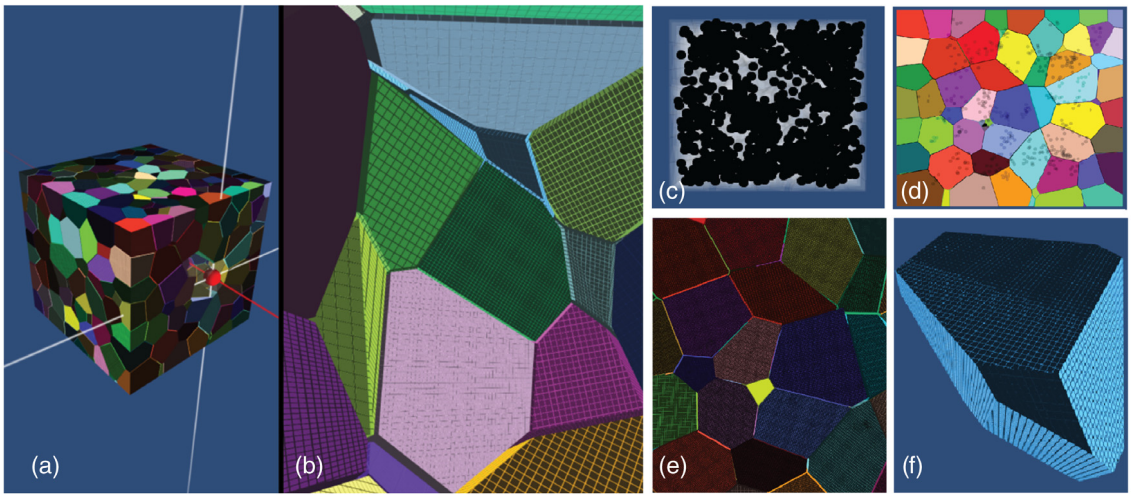

Fig. 10. Screenshots of multiscale interactive prototype. System setup (a, b): situation map, viewing area. Grain representation changes as a function of user distance: (c) far: icon representation allows assessing grain density, (d) close: basic geometry is shown in opaque colors, (e) closer: image textures can communicate crystallographic orientation, (b) inside: the grain turns transparent in order to avoid occlusion, (f) grain selection for individual inspection. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

the Chi-Squared test, as the obtained value for X^2 corresponds to a probability of coincidence lower than 95%, which is recommended in this method, meaning that the sample cannot be considered similar to the reference from a statistical standpoint. This does not mean, however, that they are unrelated. A brief analysis indicated that the procedure suggested by Exner [17] is sensitive to differences in the curve tails, which is the case here (see Fig. 4). It should be noted that the reference curve adopted in this study also deviates from the log-normal pattern [39]. In fact, the difficulty in conforming the curve tails to the log-normal pattern is a known issue in synthetic microstructures, as reported by several authors [38,42,43]. Additionally, Zhang et al. [39] data on alpha iron was based on serial sectioning, where volume was calculated by summing the volumes of the slices, each one defined by the area average of upper and lower sections, multiplied by slice thickness. Finally, the extreme slices were assumed conical. It is argued that most of the divergence found in size distribution is probably due to different measurement methods, since the volume of digital grains obtained in this work is known and accurate. Zhang et al.'s measurement also suffers from resolution loss on grain boundaries due to metallographic attack. Still, such aspects must be further studied.

Nonetheless, the resulting distribution was considered geometrically accurate enough for learning purposes. Graphical analysis indicates proximity of curve pattern and values and it is known that Voronoi diagrams on random seeds result in normal distributions. Accordingly, the final distribution curve should be situated between a normal and a log-normal pattern. The resulting curve is way flatter than a normal curve and spreads towards the end, as it is the case with log-normal curves. Therefore, it is safe to affirm that the proximity between obtained and reference distribution curves is not due to chance.

5.2. Visualization

The original and integrated approach resulted in interesting and novel interactive tools for visual analysis of grain structures, considering the educational application field. Preliminary testing suggests that dynamic real-time sectioning has superior learning value as improved spatial comprehension compared to similar earlier attempts [2] on conventional 3D visualizations but especially to available educational options such as static sections. As testing for learning improvements possibly caused by the introduction of a new tool is onerous and demands time, the hypothesis for this study is that improving the detection or experience of relevant features will improve learning, especially if this tool fits educational requirements such as a fast learning curve and high usability. Participants found the tool compelling, accessible, simple to use and learn. The tool allowed detecting in a brief period of time fundamental microstructural characteristics such as grain size and shape by translation and rotation movements while fluid continuous interactive navigation along the sample allowed participants to get a good sense of the structure and to discover spatial heterogeneities such as big or small grain clusters. Task 4 results have shown that participants were able to properly understand the concept of heterogeneity. Although they had limited knowledge on grain structures, most agreed that interactive sectioning provided a unique spatial experience of grain structures, given available possibilities for students such as single sections images or microscopes. Two interesting testimonials were: "typical superficial images observed on microscopes do not allow having a volumetric sense of the grains, which the interaction sectioning permitted"; "One reason for my motivation was curiosity to 'discover' how grains really looked like".

It is clear that the interaction leverages advantages of traditional sections and surpasses limitations associated to the static nature that can easily mislead students, i.e., a single section tells little about the properties of any single grain but real-time sectioning can tell much about the geometric properties of the whole sample. In fact, participants' comments and Task 2 results reinforced the inherent limitations of discrete sections, particularly in the identification and characterization of smaller grains, where finer and controllable continuous movements allow for better recognition. Although no direct comparison was made with animations or conventional 3D visualization, it is pretty clear that the sectioning tool allows better and a faster focused experience of relevant learning features of grain structures, as participants were given only 5 minutes to learn the tool. High proficiency is required to perform the suggested basic visualizations (Section 4.4.1) and much more to create animations on 3D software such as Blender, which conflicts with educational requirements. However, it is clear that spatial ability, navigation proficiency and motivation are strongly related to performance. The absence of spatial references reflected the predicted difficulties in locating inside the sample or in estimating rotations and is probably related to the reported cognitive overload and limited spatial ability of some participants.

Therefore, the introduction of such referential features and a little extra time to get used to the navigation commands will improve model experience for students with less spatial abilities. In fact, more time spent on such an interactive tool is an effective way to effectively train this skill [44].

Despite that interactive sectioning seems a good and simple choice, it still has some limitations, that can be addressed by other features demonstrated here. As suggested by the literature and the user study, multiscale models of grain structures promise to build stronger comprehension bridges across scales. Visual design was also explored to some extent, as recommended by [28], which helps in boosting motivation. The GC tool was found to be visually appealing and design features were directly related to high value visual analysis capabilities, such as easier visibility control and intuitive visualization of local grain density, recalling that occlusion and object crowding are inherent limitations of sectioning. Therefore, despite the positive results obtained so far, such methods still need further improvements, consolidation and comparative user testing to prove which one is better for the intended application and confirm superiority over other learning resources. Those methods may also improve cognition of other microstructural features, although they were based on fundamental characteristics of grains. Finally, the assumption of good spatial ability of engineering students must be fully assessed and students from related areas must be included in the testing procedures.

Sufficient model fidelity was pursued to avoid creating false perceptions of geometric and topological features of grain structures. Surface appearance is simplified in the current models, for instance. Since grain models are not widely used for education and interactive methods for visual analysis of grain structures are still lacking, the priority is to explore simplified models first. Simpler models can be explored for educational purposes as is the case of the ideal energetically balanced grain structure, composed of single sized grains that can be created by a Voronoi tessellation based on a perfect square point grid, producing identical tetracaidecahedral grains and a vertical distribution 'curve'. Still, in order to reproduce the organic appearance of real grains, random or intentional surface irregularities can be imposed on the flat surfaces using built-in geometry functions—an example of this was already demonstrated (Fig. 8e, f, g). However, achieving smooth surfaces can lead to a hundred-fold increase in data or more due to additional triangles but the multiscale methods presented here – some of them already available in game engines – can handle resolution variation in real-time.

Other spatial scales were not explored in the multiscale prototype yet but the same algorithms apply to balance detail and volume, given that the quantity of visible objects on the scene is controlled, which is a governing factor in computing time. Currently all available objects are loaded on the scene. As soon as more scales are added, the quantity of objects will escalate and methods such as scene partitioning will be required to load and discard objects on demand. The combination of such methods will permit computational load control by scale transitions.

6. Conclusion

An integrated approach from geometric modeling to visual analysis of digital grain structures was presented in this work, adopting an open source and comprehensive CAD platform (Blender 3D) that has robust built-in interactive visualization features and a friendly Python API. Such features clearly ease functionality extension and creation as demonstrated on new interactive functionalities. In this sense, aside from research applications, this method can also provide teachers and students seamless access to grain structure geometric modeling and interactive visual analysis capabilities, which is an empowerment resource in educational and scientific training environments, given the costs and accessibility challenges commonly associated with simulation software.

The proposed modeling method combines in a novel manner physics-based particle packing with traditional Voronoi tessellations. An interesting novel technique was devised to deal with known Voronoi distortions on grain size distribution. Samples were produced in good agreement with alpha iron data obtained directly in three dimensions, in terms of grain geometry and size distribution. The method is considerably fast compared to others, an interesting feature for applications that demand ample models. Microstructural models up to 1050 grains were produced in less than a minute, already in polygonal form and structured for direct use in game engines. The method is not as accurate as the standard simulated annealing but approximation methods are typically developed in computer graphics to achieve proper interaction and visualization speeds in novel applications. Finally, the interactive character might appeal to several applications that demand human reasoning of the process or direct intervention. In this sense, the synthesis method proposed here is considered a meaningful technical contribution. Considering that interactive visual analysis of grain structures is in its infancy and proper models and methods are still needed, polygonal structured models such as the ones created in this work can be readily imported and explored in any traditional CAD software or game engines.

Novel tools demonstrated in this paper sought to advance interaction and visual analysis methods for digital grain models, tackling a relatively untouched knowledge domain to answer a relevant need. This unique proposal adopts computer graphics and virtual reality technologies and methods in a visual analytics paradigm to enhance learning of grain structures. Preliminary testing indicates that the interactive sectioning tool is a good starting choice for improving visual analysis of grain structures in a practical and simple way in educational contexts, supporting students in deciphering relevant grain structures spatially, either individual grain characteristics such as size and shape or sample characteristics as well, such as heterogeneities in grain density. Other promising analytical features such as manual and automatic filtering, alternative simultaneous representations, including transparency, wireframe, icons, 'see-through' geometry, voxelized boundaries and multiscale features will improve limitations of interactive sectioning. The next step is to choose, combine and integrate these prospective visual analysis tools and evaluate the results on larger comparative formal user experiments. Still, several fruitful combinations for better cognition of hermetic geometric structures were already demonstrated.

Acknowledgments

This research was funded by CNPq (grant 485436/2012-4) and CAPES (grant 2993/2013).

Appendix A. Supplementary data

Supplementary material related to this article can be found online at http://dx.doi.org/10.1016/j.cad.2017.11.001.

References

[1] Fischer M, Lutomski P, Stieben A, Bleck W. 3D metallography of multiphase steels. In: Charact. miner. met. mater.. Hoboken, NJ, USA: John Wiley & Sons, Inc.; 2012. p. 175–84. http://dx.doi.org/10.1002/9781118371305.ch22.

[2] Lanzagorta M, Kral MV, Swan JE, Spanos G, Rosenberg R, Kuo E. Three-dimensional visualization of microstructures. In: Proc Vis '98 (Cat No98CB36276). Vol. 98. 1998. p. 487–90. http://dx.doi.org/10.1109/VISUAL.1998.745350.

[3] Hornbogen E. A systematic description of microstructure. J Mater Sci 1986;21:3737–47. http://dx.doi.org/10.1007/BF00553424.

[4] DeHoff RT. Microstructology: The realistic and quantitative description of microstructural evolution. Metallogr Microstruct Anal 2012;1:244–58. http://dx.doi.org/10.1007/s13632-012-0042-8.
[5] Huk T. Who benefits from learning with 3D models? the case of spatial ability. J Comput Assist Learn 2006;22:392–404. http://dx.doi.org/10.1111/j.1365-2729.2006.00180.x.
[6] Byrne CM. Water on tap: The use of virtual reality as an educational tool. University of Washington; 1996.
[7] Alias M. Spatial visualisation ability and problem solving in civil engineering. University of Surrey; 2000.
[8] Khvilon E, Patru M. Information and communication technologies in teacher education: A planning guide. UNESCO; 2002.
[9] Groeber MA, Jackson MA. DREAM.3D: A digital representation environment for the analysis of microstructure in 3D. Integr Mater Manuf Innov 2014;3:5. http://dx.doi.org/10.1186/2193-9772-3-5.
[10] Quey R, Dawson PR, Barbe F. Large-scale 3D random polycrystals for the finite element method: Generation, meshing and remeshing. Comput Methods Appl Mech Engrg 2011;200:1729–45. http://dx.doi.org/10.1016/j.cma.2011.01.002.
[11] Sintay SD. Statistical microstructure generation and 3D microstructure geometry extraction. Carnegie Mellon University; 2010.
[12] Sakurai K, Miyata K. Modelling of non-periodic aggregates having a pile structure. Comput Graph Forum 2014;33:190–8. http://dx.doi.org/10.1111/cgf.12266.
[13] Peytavie A, Galin E, Grosjean J, Merillou S. Procedural generation of rock piles using aperiodic tiling. Comput Graph Forum 2009;28:1801–9. http://dx.doi.org/10.1111/j.1467-8659.2009.01557.x.
[14] Jagnow R, Dorsey J, Rushmeier H. Stereological techniques for solid textures. ACM Trans Graph 2004;23:329. http://dx.doi.org/10.1145/1015706.1015724.
[15] Romanova VA, Soppa E, Schmauder S, Balokhonov RR. Mesomechanical analysis of the elasto-plastic behavior of a 3D composite-structure under tension. Comput Mech 2005;36:475–83. http://dx.doi.org/10.1007/s00466-005-0682-5.
[16] Underwood EE. Quantitative stereology for microstructural analysis. Microstruct Anal Tools Tech 1973;V:35–66.
[17] Exner HE. Analysis of grain- and particle-size distributions in metallic materials. Int Mater Rev 1972;17:25–42.
[18] Kumar S, Kurtz SK. Simulation of material microstructure using a 3D voronoi tesselation: Calculation of effective thermal expansion coefficient of polycrystalline materials. Acta Metall Mater 1994;42:3917–27. http://dx.doi.org/10.1016/0956-7151(94)90170-8.
[19] Mao Y, Gokhale AM. Computer simulations of realistic three-dimensional microstructures of discontinuously reinforced aluminium alloy composites. Int J Comput Mater Sci Surf Eng 2013;5:322. http://dx.doi.org/10.1504/IJCMSSE.2013.059123.
[20] Du Q, Wang D. Tetrahedral mesh generation and optimization based on centroidal Voronoi tessellations. Internat J Numer Methods Engrg 2003;56:1355–73. http://dx.doi.org/10.1002/nme.616.
[21] Siiriä S, Yliruusi J. Particle packing simulations based on Newtonian mechanics. Powder Technol 2007;174:82–92. http://dx.doi.org/10.1016/j.powtec.2007.01.001.
[22] Basanta D, Miodownik MA, Holm EA, Bentley PJ. Using genetic algorithms to evolve three-dimensional microstructures from two-dimensional micrographs. Metall Mater Trans A 2005;36(7):1643–52.
[23] Zhou Y, Huang H, Wei L-Y, Wang R. Point sampling with general noise spectrum. ACM Trans Graph 2012;31:1–11. http://dx.doi.org/10.1145/2185520.2335427.
[24] Donev A, Stillinger FH, Chaikin PM, Torquato S. Unusually dense crystal packings of ellipsoids. Phys Rev Lett 2004;92:255506. http://dx.doi.org/10.1103/PhysRevLett.92.255506.
[25] Ma C, Wei L-Y, Tong X. Discrete element textures. In: Proc. of ACM SIGGRAPH'11; 2011. p. 1. http://dx.doi.org/10.1145/1964921.1964957.
[26] Benedetti I, Aliabadi MH. A three-dimensional grain boundary formulation for microstructural modeling of polycrystalline materials. Comput Mater Sci 2013;67:249–60. http://dx.doi.org/10.1016/j.commatsci.2012.08.006.
[27] Kumar S, Kurtz SK, Agarwala VK. Micro-stress distribution within polycrystalline aggregate. Acta Mech 1996;114:203–16. http://dx.doi.org/10.1007/BF01170404.
[28] Swan JE. Visualization needs more visual design!. In: Proc. vis. '99 (Cat. 99CB37067). IEEE; 1999. p. 485–90. http://dx.doi.org/10.1109/VISUAL.1999.809939.
[29] Ullah A, Liu G, Wang H, Khan M, Khan DF, Luan J. Optimal approach of three-dimensional microstructure reconstructions and visualizations. Mater Express 2013;3:109–18. http://dx.doi.org/10.1166/mex.2013.1108.
[30] Kaufman A, Mueller K. Overview of volume rendering. In: Vis. handb.. 2005. p. 127–74. http://dx.doi.org/10.1016/B978-012387582-2/50009-5.
[31] Crassin C, Neyret F, Lefebvre S, Eisemann E, Sophia-antipolis I. GigaVoxels: Ray-guided streaming for efficient and detailed voxel rendering. In: ACM SIGGRAPH Symp Interact 3D Graph Games. Vol. 1. 2009. p. 15–22. http://dx.doi.org/10.1145/1507149.1507152.
[32] ALICE: Geometry and Light an ICG project-team. Graphite n.d. http://alice.loria.fr/index.php/software/3-platform/22-graphite.html (accessed 06.08.17).
[33] Joy KI. Massive data visualization: A survey. In: Möller T, Hamann B, Russell RD, editors. Math. found. sci. vis. comput. graph. massive data explor.. Berlin, Heidelberg: Springer Berlin Heidelberg; 2009. p. 285–302. http://dx.doi.org/10.1007/b106657_15.
[34] Smelik RM, Tutenel T, Bidarra R, Benes B. A survey on procedural modelling for virtual worlds. Comput Graph Forum 2014;33:31–50. http://dx.doi.org/10.1111/cgf.12276.
[35] Doškář M, Novák J. A jigsaw puzzle framework for homogenization of high porosity foams. Comput & Structures 2016;166:33–41. http://dx.doi.org/10.1016/j.compstruc.2016.01.003.
[36] Ghosh S, Bhandari Y, Groeber M. CAD-based reconstruction of 3D polycrystalline alloy microstructures from FIB generated serial sections. Comput Des 2008;40:293–310. http://dx.doi.org/10.1016/j.cad.2007.11.003.
[37] blender.org. blender.org - Home of the Blender project - Free and Open 3D Creation Software. Blender.org 2015. https://www.blender.org/ (accessed 13.03.17).
[38] Donegan SP, Tucker JC, Rollett AD, Barmak K, Groeber M. Extreme value analysis of tail departure from log-normality in experimental and simulated grain size distributions. Acta Mater 2013;61:5595–604. http://dx.doi.org/10.1016/j.actamat.2013.06.001.
[39] Zhang C, Suzuki A, Ishimaru T, Enomoto M. Characterization of three-dimensional grain structure in polycrystalline iron by serial sectioning. Metall Mater Trans A 2004;35:1927–33.
[40] Spettl A, Wimmer R, Werz T, Heinze M, Odenbach S, Krill III CE, Schmidt V. Stochastic 3D modeling of Ostwald ripening at ultra-high volume fractions of the coarsening phase. Model Simul Mater Sci Eng 2015;23:65001. http://dx.doi.org/10.1088/0965-0393/23/6/065001.
[41] Rycroft CH. VORO++: A three-dimensional Voronoi cell library in C++. Chaos 2009;19:. http://dx.doi.org/10.1063/1.3215722.
[42] Tucker JC, Chan LH, Rohrer GS, Groeber MA, Rollett AD. Tail departure of log-normal grain size distributions in synthetic three-dimensional microstructures. Metall Mater Trans A 2011;43:2810–22. http://dx.doi.org/10.1007/s11661-011-0851-4.
[43] Krill III CE, Chen L-Q. Computer simulation of 3-D grain growth using a phase-field model. Acta Mater 2002;50:3059–75. http://dx.doi.org/10.1016/S1359-6454(02)00084-8.
[44] Sorby SA. Educational research in developing 3-D spatial skills for engineering students. Int J Sci Educ 2009;31:459–80. http://dx.doi.org/10.1080/09500690802595839.