# In de verdediging

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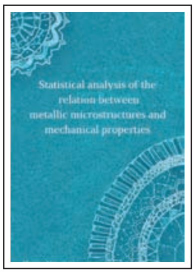



**Statistical Analysis of the Relation Between Metallic Microstructures and Mechanical Properties**
*Martina Vittorietti*

In July 2020 Martina Vittorietti from the Delft University of Technology successfully defended her PhD thesis with the title *Statistical Analysis of the Relation Between Metallic Microstructures and Mechanical Properties*. Martina carried out her research under the supervision of prof. dr. ir. G. Jongbloed, and prof. dr. ir. J. Sietsma.

During her PhD Martina developed methods that can be used to test whether a real steel microstructure can be simulated by a specific stochastic model. Following two different approaches, according to the use or not of periodic boundary conditions, Martina proposed three different model tests. Furthermore, relying on stochastic models Martina studied the relations between the intricate 3D features of metallic microstructures and the mechanical properties of the corresponding material.

At the moment Martina is a postdoc at the Delft University of Technology in the DENS project (Digitally Enhanced New Steel Product Development). This project involves more than ten PhD students and postdocs which work closely together at Tata Steel Europe, Delft University of Technology, Eindhoven University of Technology, University of Twente and the Max Planck Institut für Eisenforschung in Düsseldorf (Germany). The aim of the project is to develop a fitting computational model to shorten the time to market without compromising the quality of the steel. In her postdoc Martina plans to further extend the work done during her PhD, considering dynamic models for representing the evolution of microstructures during (virtual) mechanical tests.

## Microstructural features and mechanical problems

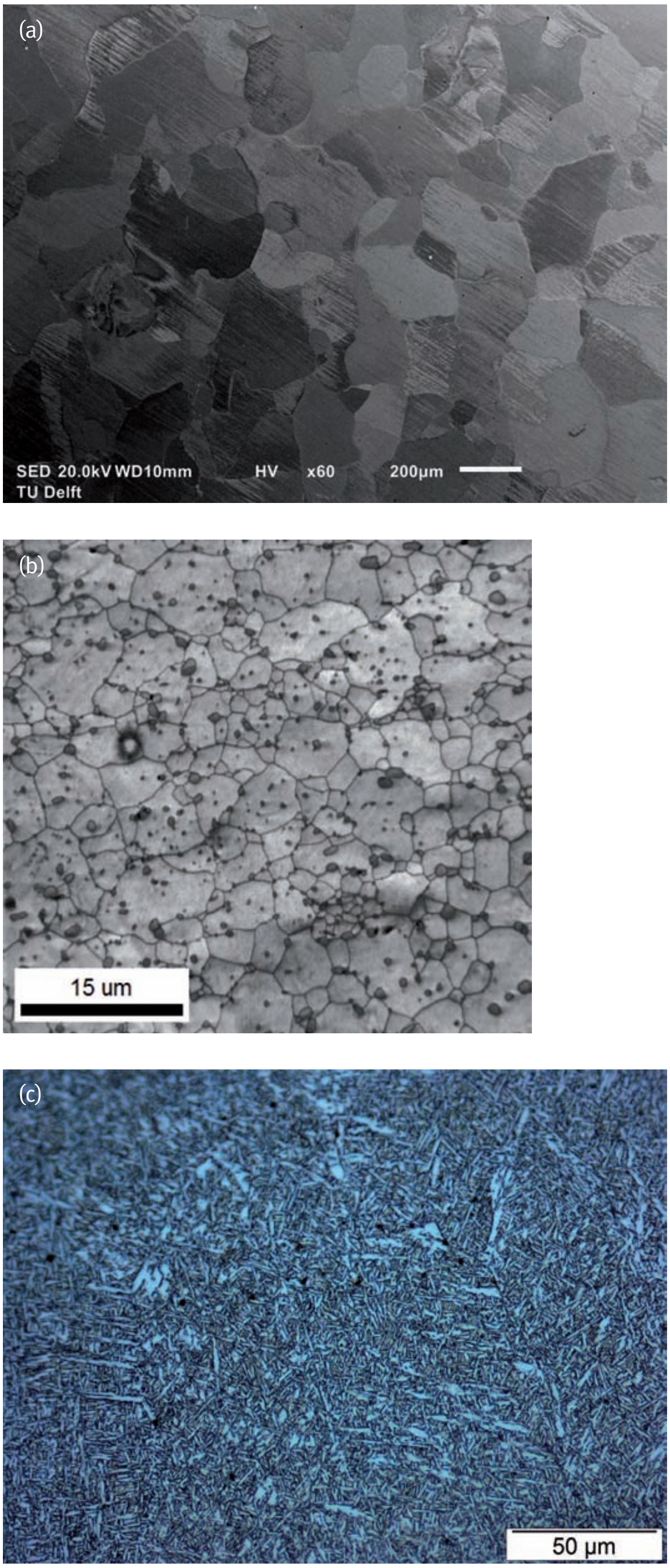
Starting from the atomic scale, metals can be described as regular aggregations of atoms held together by *metallic bonds*. Atoms form symmetrical three-dimensional aggregations which are characterized by a so-called unit cell. The unit cell completely reflects the symmetry and structure of the entire crystal, which is built up by repetitive translation of the unit cell along its principle axes.

Microstructure is the very small scale structure of a material, defined as the structure of a prepared surface of material as revealed by an optical microscope above $25\times$ magnification. Metallic microstructures usually contain more than one crystal, of one or multiple phases, with a specific orientation and possible imperfections or defects. These phases have different properties and in general, various mechanical properties of the material depend on them. For example the strength, toughness, ductility, hardness, corrosion resistance and so forth. Examples of different metallic microstructures are shown in Figure 1.

*Pas gepromoveerden brengen hun werk onder de aandacht. Heeft u tips voor deze rubriek of bent u zelf pas gepromoveerd? Laat het weten aan onze redacteur.*

*Redacteur: Nicolaos Starreveld*
*FNWI, Universiteit van Amsterdam*
*Postbus 94214*
*1090 GE Amsterdam*
*verdediging@nieuwarchief.nl*

Metaphorically speaking one can say that the microstructure forms the DNA of materials and hence contains all the necessary information determining their properties. Ideally, being able to *genetically modify the DNA* of the material means that it is possible to obtain a product with some desired properties. For example, materials such as Advanced High-Strength Steels (AHSS) are of great interest for high-tech applications because of their higher strengths compared to conventional steels. In the automotive industry this higher strength enables lightweight, fuel-efficient designs, which are also safer than those using conventional materials. In order to develop new AHSS, and more generally new materials, steel industries make use of multi-scale microstructure modelling to predict mechanical properties from information about the microstructure. Unfortunately, in reality the quantitative identification of the relation between microstructural features and mechanical properties is very hard..




Illustrations: Wei Li, Javier Hidalgo and Aravind Babu

**Figure 1** (a) Single-phase steel microstructure, (b) AISI stainless steel with M_23C_6 carbides precipitation (two phases), (c) Multi-phase steel microstructure.

During her PhD Martina developed statistical techniques that make it possible to infer relations between the intricate 3D features of metallic microstructures and the mechanical properties of the corresponding material.

## Poisson–Voronoi diagrams

The most common technique to gather microstructural information is by analysing 2D images taken using suitable tools, such as optical microscopes or electron microscopes. This means that an intrinsically three-dimensional object is reduced to a two-dimensional plane. This can also be viewed as a statistical problem, considering that the 2D picture must be a representative sample of the 3D microstructure. We will refer to this as the representation problem. The aim is to gather in one 2D image all the characteristic features of the microstructure and then relate them to the original 3D structure. In her research Martina used microstructural modelling relying on Poisson–Voronoi diagrams to simulate the behaviour of multi-phase microstructures.

### *3D Poisson–Voronoi diagrams*

Intuitively, for defining a 3D Poisson–Voronoi diagram, a random set of points (also called generator points, sites or nuclei) is generated in a finite volume. Afterwards spheres having these points as centres are grown at the same time and with the same speed; once two spheres touch a face between them appears. This results in a space-filling configuration made of convex polyhedra, also called cells or grains. In the Poisson–Voronoi diagram the nuclei, or sites, are generated by a homogeneous Poisson process with intensity parameter $\lambda$. Poisson–Voronoi diagrams are suitable when studying single-phase microstructures, see Figure 1(a), but not so suitable when studying multi-phase microstructures, Figure 1(b,c). In order to study multi-phase microstructures Tata Steel developed an algorithm based on the generation of a so-called Multi-Level Poisson–Voronoi diagram. A visualization of such a diagram is shown below in Figure 2, for the exact definition the interested reader can have a look at Martina's thesis.

(Multi-level) Poisson–Voronoi diagrams have been commonly employed for representing (multi-)single-phase steel microstructures. More specifically, Martina used Multi-level Poisson–Voronoi diagrams to represent the microstructure of AISI420 stainless steel with M_23C_6 carbides, Figure 1(b), and Figure 3 below. A challenging statistical question that arises is whether Poisson–Voronoi diagrams offer an adequate microstructure model, given the data observed from the 2D images. We will refer to this question as the *Poisson–Voronoi assumption*.

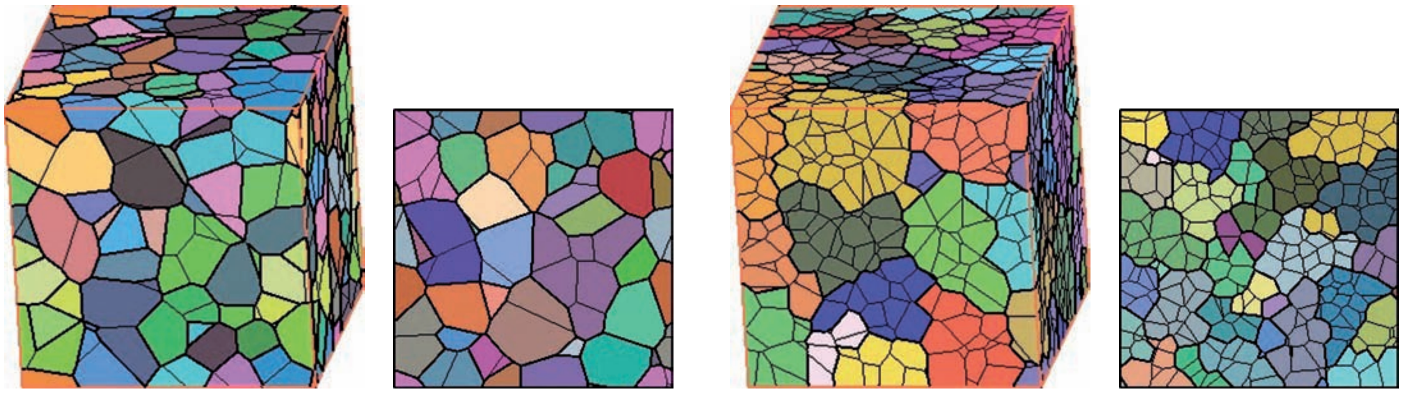


**Figure 2** 3D Multi-Level Poisson–Voronoi diagrams and corresponding 2D sectional Multi-Level Poisson–Voronoi diagrams with different intensity parameters.

### Where there Is matter there is statistics

In her PhD Martina developed a general framework for testing the Poisson–Voronoi assumption based on images of two dimensional sections of real metals. Martina extended already existing statistical tests including more accurate measures based on recently developed tools provided by Topological Data Analysis. In cases in which the Poisson–Voronoi diagram hypothesis is rejected then more complex models have to be developed and used.

Besides the representation problem Martina also worked on the mechanical problem, which concerns the inference of mechanical properties of the material given information on the microstructure. To give an example, strain development in metallic alloys is critically affected by the microstructural characteristics. In her thesis Martina investigated the properties of a AISI420 stainless steel with M_23C_6 carbides precipitates, see Figure 1(b).

For this she performed a virtual tensile test. The basic idea of such a test is to firstly generate a so-called digital twin microstructure on which a virtual tensile test is performed. In order to create the digital twin microstructure for this specific material Martina used a Multi-level Poisson–Voronoi diagram with two phases. Then, the virtual tensile test was performed using a program called DAMASK. The Düsseldorf Advanced Material Simulation Kit (DAMASK) is an open source software based on a Crystal Plasticity methods which allows to conduct advanced microstructural and mechanical property simulations. The main outcomes of the experiments are stress-strain curves corresponding to the different microstructures.

The most commonly used test is the uniaxial tensile test in which force is applied to the test sample with respect to just one specific axis causing deformation of the material, temporarily (elastic behaviour) and permanently (plastic behaviour) and eventually its fracture. Tensile testing is one of the most common ways for investigating strength, ductility and in general loadability (the ability of a material to support a stress) of metallic materials. Martina's virtual experiments suggest that as the concentration of M_23C_6 carbides increases the metallic material becomes more resilient to high stress.

### The more personal aspect

Behind all dissertations there is always a person, with flesh and bones, who has endured the long path of a PhD trajectory and has produced the work at hand.

*Were you also involved in some other activities and events during your PhD?*

"I've been an organiser of the PhD seminar for the Probability and Statistics group of the department of Applied Mathematics of Delft University of Technology. During my PhD I also kept working on my Master Thesis project with my previous university, University of Palermo, on a different area: Social Statistics.

And something not related to research, I was the organiser of the PhD Christmas party. I love the cultural diversity that you encounter in the department of applied mathematics of TU Delft. Therefore, some days before Christmas holiday, I was asking all the PhD's of the department to join the Christmas party bringing something to eat or drink (preferably typical dish of their country) and did my best to persuade them to wear something red. The party was 'secret' but everybody started to suspect when everybody was wearing red."

*Are there some nice memories from the last four years you would like to share?*

"I remember the day in which I received the call from the HR department of TU Delft to arrange the Skype interview for the PhD position. It was the day of my Master graduation and I was celebrating with my family and friends. At one point my phone started to ring and I saw that the call was from The Netherlands. So I asked everybody to keep quiet and I answered the phone. When I heard that they were interested in interviewing me I was doubly happy."

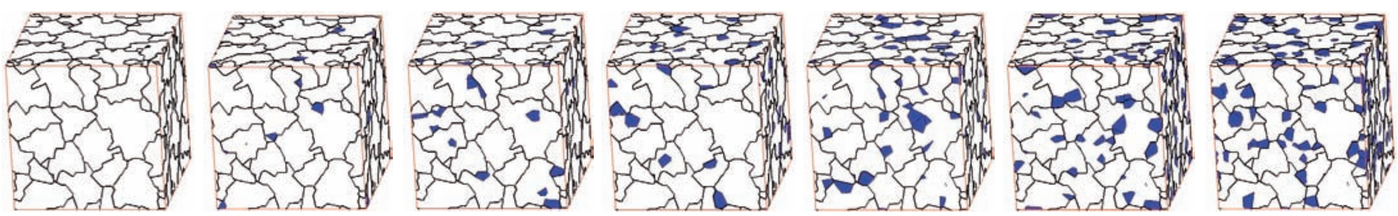


**Figure 3** 3D Multi-Level Poisson-Voronoi diagram with two phases that Martina used to represent the microstructure of AISI420 stainless steel with M_23_C6 carbides, from left to right the intensity of the parameter corresponding to the M_23C_6 carbides is increased.