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Introduction

TATB (1,3,5-triamino-2,4,6-trinitrobenzene) is an energetic molecular crystal that combines high energetic performance and good thermal stability. By adding a small amount of a polymer acting as a binder between TATB grains, it is possible to obtain exceptionally safe explosives displaying good mechanical properties. A first step toward the understanding of the influence of the microstructure on the mechanical properties of TATB is the development of stochastic models to describe the microstructure of the material.

Materials and Methods

In a previous work, Ambos *et al.* [1] developed a model based upon Johnson-Mehl tessellations [2]. This model afforded curved grain boundaries, and therefore a certain non-convexity of grains. However, it did not reproduce their elongated character. To improve this aspect, we rely on an anisotropic Johnson-Mehl model to simulate the TATB microstructure. The Johnson-Mehl tesselation is a sequential version of the Voronoï tessellation, where nucleation germs are implanted sequentially with time. All classes grow then isotropically with the same rate, and the growth of crystal boundaries is stopped when they meet. All Poisson points falling in an existing crystal are removed. From a mathematical perspective, a Johnson-Mehl tessellation is constructed from a sequential Poisson point process where the points x_i, $i = 1, .., N$ are implanted sequentially at a time t_i, $i = 1, .., N$. The classes C_i, $i = 1, .., N$ corresponding to the points x_i, $i = 1, .., N$ are defined by

$$C_i = \left\{ y \in \mathbb{R}^3, \forall j \neq i, t_i + \frac{\|x_i - y\|}{v} \leq t_j + \frac{\|x_j - y\|}{v} \right\}.$$

In our study, we introduce a modified version of the Johnson-Mehl model. Our aim is to account for the shape anisotropy of the grains. To that end, we attach to each implanted point a random direction taken on the unit sphere S^3, which will be referred to as principal growth direction, thus forming a marked point process P in $\mathbb{R}^3 x S^3 x \mathbb{R}+$. All points of P are then implanted sequentially with time. Once a point is implanted, the corresponding class grows with an orientation-dependent velocity, defined for all vector **u** of the unit sphere S^3 by

$$\mathbf{V}(\mathbf{u}) = \mathbf{u} + (K - 1)(\mathbf{u}.\mathbf{p})\,\mathbf{p}$$

where **p** denotes the principal growth direction and **u.p** is the scalar product between vectors **u** and **p**. K is a parameter introduced to model grain anisotropy.

Results and Discussion

Overall, the model is characterized by two parameters, namely the intensity θ of the nucleation process and the anisotropy factor K. In our study, the sample image of the material provides us with a bidimensional section of the tridimensional microstructure. Estimating the parameters of the model is thus a complicated task, especially since in practice, stereological properties of the anisotropic Johnson-Mehl model are hardly tractable analytically [3, 4]. As a consequence, we rely on the minimum contrast method to perform the parameters estimation [5]. Our approach consists in selecting the model parameters that minimize the difference between the granulometry and the distribution of eccentricities of the grains of the tessellation as measured on the sample image and on the random realizations. We rely on the Nelder-Mead algorithm [6] to perform the parameters identification. The optimal couple of parameters is found to be $\theta = 5.0 \times 10^{-7}$ $\mu m^{-3}/s$ and K = 2.24 and is illustrated in Figure 1. Figure 2 compares the predicted and experimental two-dimensional grain size and elongation distributions.

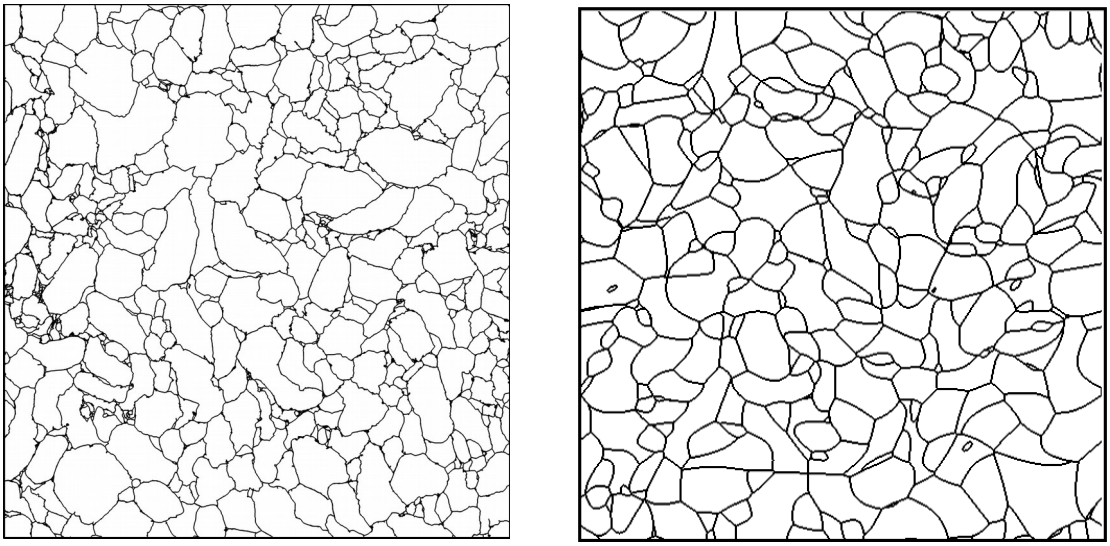

Figure 1. Experimental (left) and simulated (right) images of a slice of the tri-dimensional crystaline microstructure.

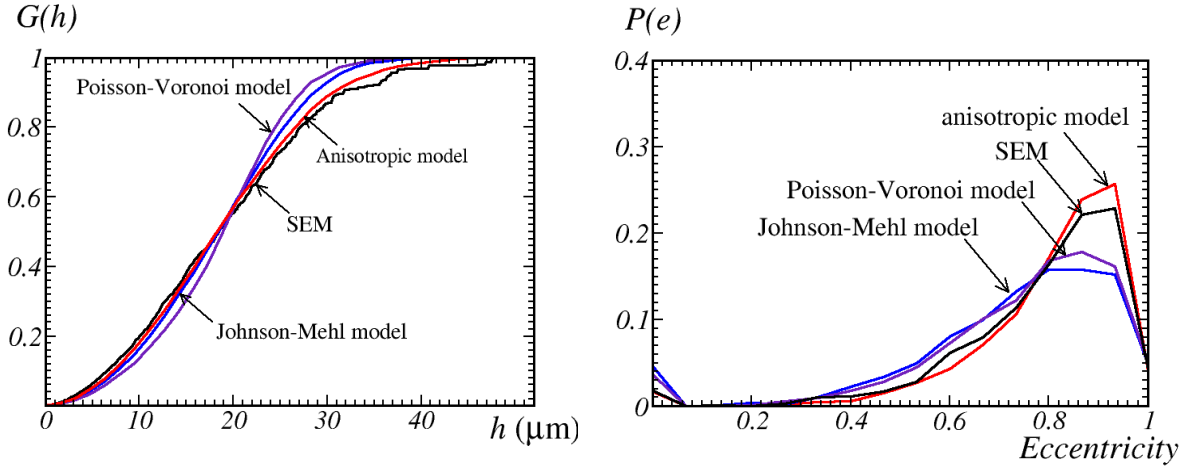

Figure 2. Granulometries (left) and grains eccentricities distribution (right) of the simulated microstructures for distinct models, compared with the one measured on the sample image of the microstructure.

Conclusion

In this study, we developed a stochastic model aimed at describing the complex crystalmicrostructure of TATB crystal. The model is based upon a Johnson-Mehl tessellation with anisotropic distance, which allows us to capture the grain anisotropy. The result appears quite satisfactory, except for the smallest grain fraction, say below 10 μm.

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