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Effect of the random spatial distribution of nuclei on the transformation plasticity in diffusively transforming steel

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Abstract: The $\gamma \rightarrow \alpha$ diffusive phase transformations of steels can lead to transformation plasticity (TRIP) if accompanied of an external loading stress or a pre-hardening of the parent phase. The most current approaches of its modelling are based on the Greenwood-Johnson mechanism; they call upon hypotheses (about microstructure morphology, constitutive laws...) which are at the origin of discrepancies between predictions and experimental observations in particular loading cases. Some of these restricting hypotheses can be eliminated with a micromechanical finite elements approach, where the elastoplastic interactions between phases are determined at the micro-scale of a volume element containing hundreds of growing particles (Barbe et al., 2005, 2008). This paper deals with the effect of the spatial distribution of product phase nuclei on the global kinetics and transformation-induced plasticity (TRIP) in the volume element. Two distributions are considered: uniform random and at preferential nucleation sites of a Voronoi tessellation mimicking austenite microstructure.

Keywords: transformation-induced plasticity; TRIP; Voronoi tessellation; steel diffusive transformation; nuclei random distribution; micromechanical finite-elements modeling.

1 Introduction

During the cooling diffusive transformation of steel from the austenitic domain, the product phase is usually the harder phase and also the less compact. When the material is submitted to an external load (even inferior to the yield stresses of the present phases), these two features lead to transformation-induced plasticity (TRIP). This is shown, for example, by the experimental tests performed by Taleb and Petit-Grostabussiat concerning the bainite transformation of a 16MND5 steel (used in French nuclear reactor vessels; ASTM norm: SA508C13) (Petit-Grostabussiat et al., 2004). This phenomenon is reproduced with correct accuracy by different micromechanical models [e.g., the model of Leblond (1989) and its generalisation due to Taleb and Sidoroff (2003)]. However, investigations of Taleb and Petit (2006) have shown that, when the parent phase is submitted to pre-hardening, such analytical micromechanical models do not provide satisfactory predictions. To improve modelling, it is necessary to introduce more details on the material and its transformation, that is why the present numerical micromechanical model is developed.

The model used in this work [inspired from Leblond (1989), Ganghoffer et al. (1993) and extended in Barbe et al. (2007), Hoang et al. (2007), Barbe et al. (2008) and Hoang (2008)], contrary to analytical models, does not introduce any assumption on the distribution of the mechanical fields at the vicinity of the interface between parent and product phase: the regions occupied by each phase in the volume of study being imposed, the mechanical balance in the medium is ensure all along the transformation with the finite elements (FE) method. This enables to solve the problem with any kind of elastoplastic behaviours of the phases, transformation type (and loading).

At the current state of our modelling, each phase is attributed homogeneous mechanical properties; further developments will account for the crystallographic character of the medium by using crystal plasticity constitutive laws and sub-division of the parent medium into grains [as proposed for example in Barbe et al. (2001), Nygards and Gudmundson, (2002) and Diard et al. (2005)]. The zones of product phase have a cubic morphology and grow at an imposed rate. From a mechanical point of view, the problem is an inclusion-matrix elastoplastic problem where inclusions, with compactness and elastoplastic properties different from those of the matrix, grow diffusively in the matrix and take its place. The classical case where inclusions are considered to be regularly distributed, which enables significant simplifications due to symmetries, has been analysed in details in Barbe et al. (2007). As global transformation kinetics is badly represented, the case where inclusions are distributed through a Poisson process has been the subject of Barbe et al. (2008) and the methodology has been described in details. Nevertheless, the influence of the distribution of the nuclei (uniform or with preferential sites) has not been addressed and is under concern in the present paper. Indeed, the crystalline feature of the parent phase may have an influence. To take it into account, the parent phase is modelled by a Voronoi tessellation, which is a typical representation for polycrystalline materials, and the nuclei are considered to be at the vertices of the Voronoi polyhedra (VVP). As explained in more detail in Subsection 2.2, this kind of distribution is expected to be closer to the one of real phase transformations than a poisson distribution. It is further checked that this kind of distribution really differs from a poisson distribution. In Section 3, an analysis of the effect of the spatial distribution of nuclei on global transformation kinetics and TRIP is presented. These investigations are some preliminary steps of the development of a more physically based model where the crystalline feature of the medium is taken into account.

2 Modelling

2.1 FE modelling

This subsection is a reminder of the FE modelling detailed in Barbe et al. (2005) and Barbe et al. (2007): material properties, type of finite elements, boundary conditions, loading and strain decomposition have been detailed therein.

2.1.1 FE mesh

A domain of FE computation is cubic, discretised regularly into three-dimensional 8-noded brick elements, which results in $n \times n \times n$ elements if n is the number of elements along an edge of the cube.

2.1.2 Decomposition of strain

The total strain tensor E^{tot} resulting from FE simulations, is decomposed as follows: $E^{\text{tot}} = E^{\text{el}} + E^{\text{tr}} + E^{\text{tp}}$ where E_{el} is the elastic strain due to the applied tensile stress, E^{tr} is the transformation strain and E^{tp} is the transformation plasticity that corresponds to the plastic strain provided by the FE computation. This decomposition is valid locally, at any integration point of the FE mesh, and also globally on a FE domain of computation.

2.1.3 Material properties

The medium of study is constituted of two homogeneous phases, austenite (γ) and bainite (α), which differ both in mechanical properties and compactness. The mechanical behaviours are elastoplastic: linear isotropic elasticity and linear isotropic hardening, but with different parameters. Here are all the parameters:

- young modulus and poisson coefficient: 200000 MPa and 0.3 for each phase
- yield stress: 107 MPa for austenite and 433 MPa for bainite
- hardening coefficient: 2,800 MPa for austenite and 4,500 MPa for bainite
- transformation strain (change in compactness): $E_{ii}^tr = 0.0055$ for $i = 1,2,3$;
 $E_{ij}^tr = 0$ if i differs from j

Further extensions of the modelling will take into account the crystalline character of the medium by resorting to crystal plasticity: the parent medium will be divided into polyhedra [for example VVP as in Barbe et al. (2001), Nygards and Gudmundson (2002) and Diard et al. (2005)]. The material behaviour will be described by crystal plasticity constitutive laws accounting for glide on particular slip systems, and every polyhedron, representing a grain, will be assigned a particular orientation.

2.1.4 Loading/boundary conditions

A constant tensile stress (24 MPa in the present work) is imposed to two opposite faces of the cubic FE domain all along the transformation. Each face of the domain is imposed to remain plane and parallel to its initial position.

All computations have been prepared using the microstructure generation software NePeR (NePeR, 2007) and then performed with the finite element software Zset developed at the Mines Paristech and ONERA (Besson et al., 1998, <http://www.nwnumerics.com>).

2.2 Kinetics modelling

2.2.1 Temporal description of nucleation and growth

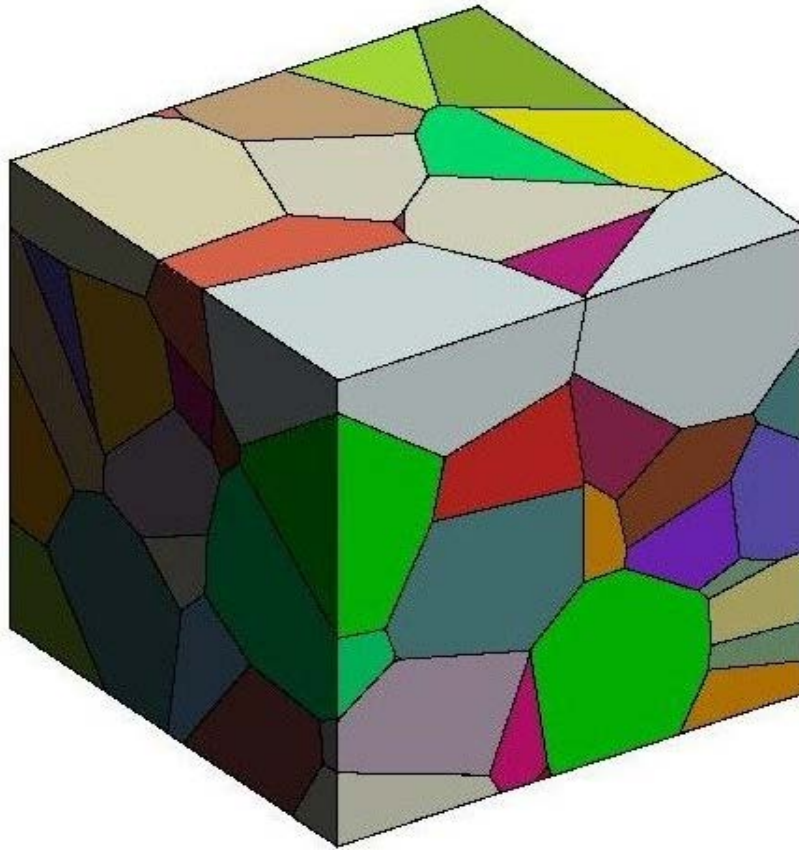
Nucleation is supposed to occur instantaneously (site-saturation hypothesis). In the extension of the modelling proposed by Hoang et al. (2007), nucleation can continue through time resulting in a temporal distribution law. Here, all the nuclei are present at the first step of transformation. At the next step, the zones of product phase grow by one element along their radii. The elements being transformed can be considered to constitute the interface between parent and product phase, and so the interface between parent and product phase is supposed to be single element wide layer. This procedure of transformation is reproduced all along the transformation, at a constant rate.

2.2.2 Spatial description of nucleation

In a general case of phase transformation, where no information is available about the microstructural morphology of the parent phase or about the preferential locations of nucleation sites in the microstructure (e.g., case of a special parent phase, notably

resulting from abnormal growth, at the opposite case of work-hardened austenite which favours intragranular nucleation), it is not possible to characterise mathematically the spatial distribution of the nuclei. In this general case of uniform probability of nucleation, the ‘largest’ randomness character is attributed to the location of the nuclei; there is absolutely no interaction rule between two nuclei. This case has been treated in details by Barbe et al. (2008).

Figure 1 Voronoi tessellation with 100 polyhedra (see online version for colours)

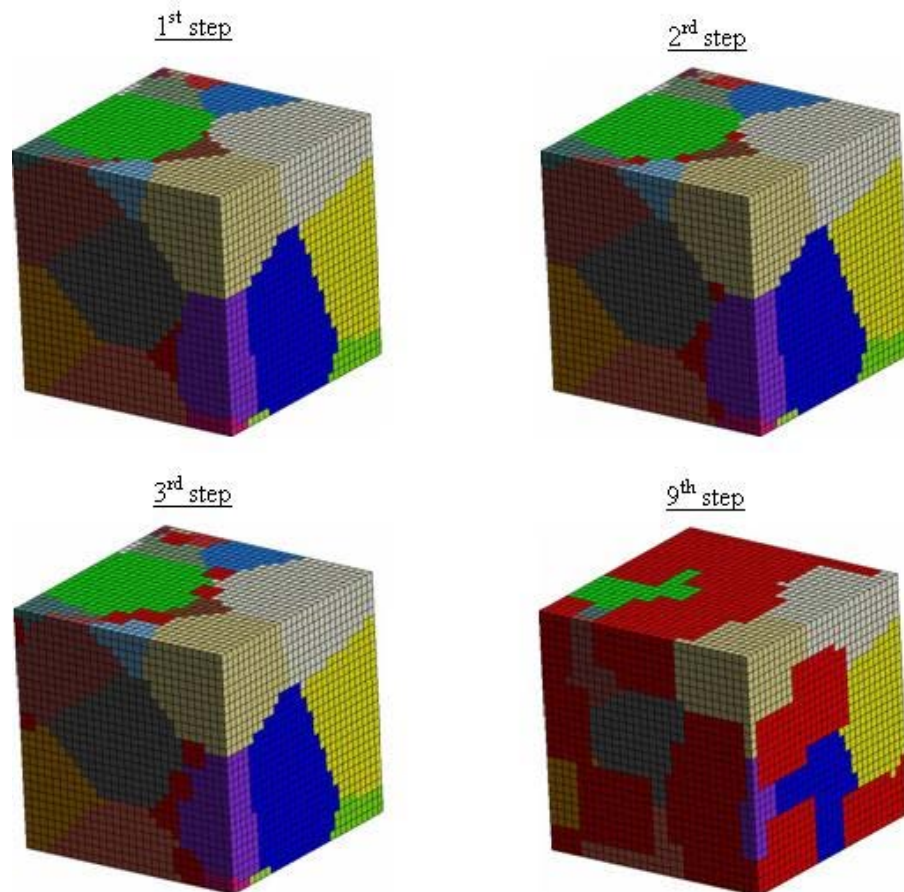


Nevertheless, in a real solid-solid diffusive transformation of steel under continuous cooling, the nuclei are often observed to appear at particular sites of the microstructure. The most favourable ones are, with decreasing proportion, the quadruple points, the triple lines, the grain boundaries (which are the intersection of 4/3/2 grains, respectively) and the grain interior. It has been shown experimentally that, in the case of an austenite to ferrite transformation of different grades of steels differing in carbon concentration, most of the nuclei appear at quadruple points (Offerman et al., 2006). To address this kind of configuration, we propose to describe the morphology of the austenite parent phase by a Voronoi tessellation, as it is proposed in several models either of phase transformation (Mecozzi et al., 2006) or of plasticity of polycrystalline aggregates (Barbe et al., 2001;

Diard et al., 2005). Indeed, the construction of a Voronoi tessellation is a process of sub-division of space which has strong similarities with the process of diffusive uniform growth of crystals in metallic materials: as seen on Figure 1, it results in convex polyhedra which reproduce, at least, the random character of the microstructural morphology of a real metallic material like austenite.

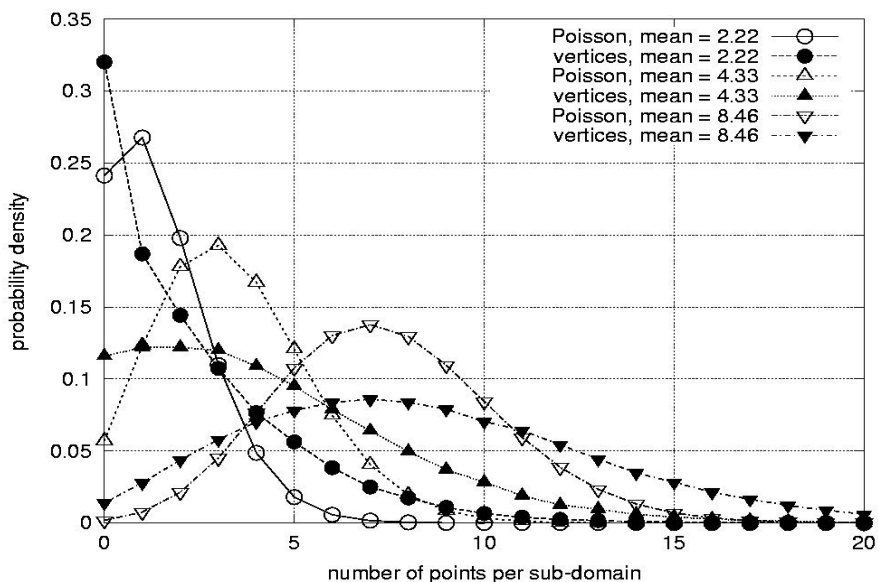
The austenite matrix being described by a Voronoi tessellation, the methodology of calculation consists in extracting sub-domains whose size is taken according to the mean number of vertices of VVP wished for the simulation of TRIP, consider the VVP as the sites of nucleation and then simulate the diffusive transformation. This process can be applied for any mesh size of sub-domains. It leads to a transformation as illustrated on Figure 2, for a sub-domain regularly meshed into 283 eight-node brick elements, where the product phase appears at the corners of the polyhedra constituting the parent phase, grows in the sub-domain, and ends up by occupying the whole sub-domain.

Figure 2 Four transformation steps in a sub-domain meshed regularly into 283 elements; the transformation starts from nuclei located at VVP (see online version for colours)



As VVP are determined bijectively from a random set of points -their centres-, the obtained vertices are randomly distributed. However, the process introduces interaction, so their spatial distribution cannot be considered to be a Poisson distribution a priori. It is a question how it differs from a Poisson distribution. To address this question for which, to our knowledge, there is no quantitative answer in the literature, we have performed a classical statistical comparison: being given a set of random points in a finite domain D , let us count the number of points found in sub-domains d taken at random locations of D . The probability $p(N)$ of finding N points, plotted as a function of N , defines the statistical distribution of N . If the coordinates of the points are defined with a uniform law of probability in D , it can be shown analytically that $p(N)$ follows a Poisson law whose parameter is the mean of N (the mean number of points per sub-domain d). For the same mean number of VVP in sub-domains d , the probability function of the VVP appears to be significantly different from the Poisson distribution. This is illustrated on Figure 3, where three different means were considered. The new distributions cannot be, to our knowledge, described by simple statistical distributions, but it is obvious that they are less uniform. The aim of the present work is to evaluate the effect of this difference on the global transformation kinetics and on TRIP

Figure 3 Probability function of finding N points in a sub-domain d for three different means of N



Note: Points are defined either with a uniform law of probability (Poisson distribution) or as VVP.

3 Analysis

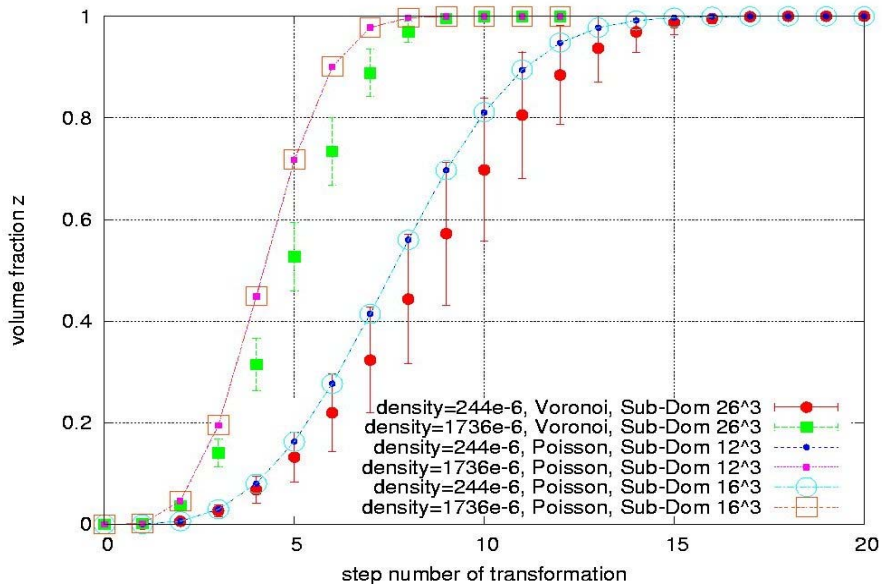
The analysis consists in comparing the results obtained in the configuration of

- 1 Poisson distribution of nuclei
- 2 nucleation at the VVP.

Two cases of nuclei density are considered: $244E-6$ and $1736E-6$, which define the probability of nucleation in an element of the mesh. Hence, the mean number of nuclei in a set of random realisations of FE sub-domains of a given size $n \times n \times n$ elements equals the density multiplied by n^3 . The two main results to be analysed are

- 1 the global transformation kinetics, i.e., the evolution of the volume fraction of product phase with respect to transformation steps
- 2 the TRIP, i.e., the spatially averaged microplasticity in the domain of computation.

Figure 4 Product phase volume fraction z as a function of the transformation step number for two densities of nucleation and for two kinds of nuclei distribution: Poisson or VVP (see online version for colours)



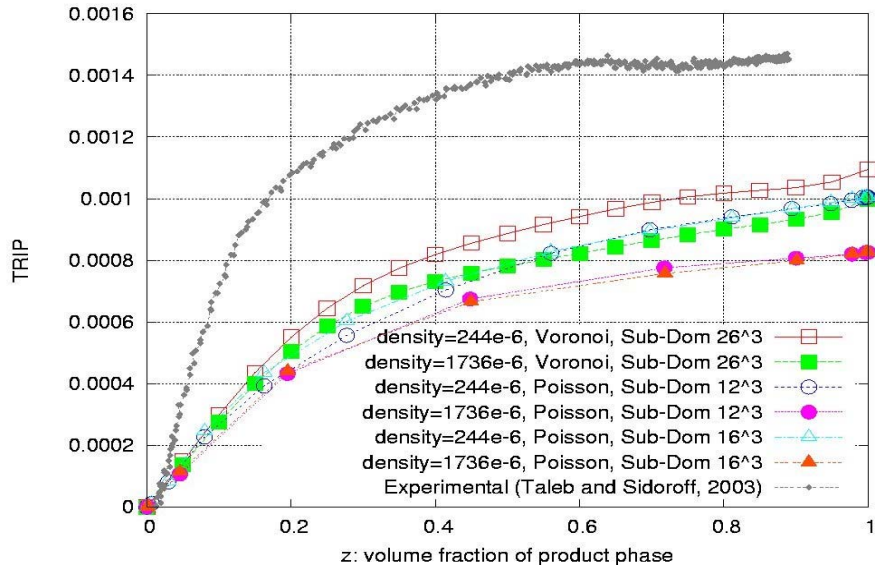
Note: Vertical error bars define the region in which all individual curves are enclosed.

As explained in Barbe et al. (2005) and Barbe et al. (2007), the global kinetics as well as the evolution of TRIP in a single realisation of FE sub domain with randomly positioned nuclei cannot be representative of effective properties unless the sub-domain is taken very large in terms of number of elements and contains a large number of nuclei. It is shown in Barbe et al. (2008) that, for nuclei densities of the order $10E-3$, even with a size of sub-domain equal to 100^3 elements, the global kinetics were significantly different from those determined analytically, relative to an infinite domain. Such a size of mesh would require about 64 CPU of a parallel machine, each with 1 Gb RAM. That is why a strategy based on ensemble averaging detailed in Barbe et al. (2008) has been used. It consists in performing the FE simulations in several sub-domains of reasonable size (typically 20^3 to 30^3 elements), which are considered to be extracted from an infinite

domain whose kinetics of nucleation and growth are known. Then, relying on the postulate of ergodicity for the medium under concern, the ensemble average over the simulated sub-domains is considered to provide the effective properties of the medium, i.e., those which would be obtained in a single representative volume element.

The global kinetics, presented on Figure 4, first show that the evolution of z for a given nuclei density and a Poisson distribution does not depend on the size of sub-domain. Along with this observation, one of the necessary conditions for the validity of the ergodicity hypothesis is being checked. The same observation should be made in the future concerning nuclei positioned at VVP. In this latter case, we observe a larger dispersion of the curves with the lower nuclei density. This means that all the more sub-domains should be used for the ensemble average that nuclei density is small. From the figure, the influence of the kind of nuclei distribution on transformation kinetics is obvious. The fact that z is lower with nuclei at VVP than with a Poisson distribution is due to the fact that, as shown on Figure 3, there are more nuclei separated by a small distance in the VVP distribution than in the Poisson distribution. Along the transformation, the impingement of growing zones appears sooner and is more pronounced.

Figure 5 TRIP as a function of volume fraction of the product phase for two kinds of nuclei distribution, two nuclei densities and different sizes of sub-domains (see online version for colours)



Note: The lines between points are only meant to ease the visualisation of the results, constituted by the points.

Concerning TRIP, plotted as a function of the product phase volume fraction on Figure 5, from a general point of view, there is a discrepancy between experimental results of Taleb and Sidoroff (2003) and the simulated curves. As shown by Hoang (2008), this is due partly to the choice of the constitutive laws describing the hardening of each phase:

for same monotonic elastoplastic behaviour, attributing a more or less importance to kinematic hardening with respect to isotropic hardening can affect the results significantly. The difference can also be attenuated by choosing a smaller nuclei density. Indeed, as can be seen on Figure 5, the smaller the density, the larger the TRIP. Concerning the Poisson distribution by itself, it is worth noting that, for a given nuclei density, TRIP does not depend on the sub-domain size. As for the global kinetics, this observation is a necessary condition to be fulfilled for the ergodicity hypothesis to be valid. Comparing the two cases of nuclei distribution, it appears that the results depend on the type of distribution, but not only because the global kinetics are different: let us compare the case of nuclei at VVP with a density $1736E-6$ to the case of a Poisson distribution with a density $244E-6$; the TRIP curve is approximately the same but the global kinetics are significantly different.

4 Conclusions

In order to describe the mechanical consequences of a solid-solid diffusive transformation occurring under external loading, and particularly the transformation induced plasticity, we use the FE method to evaluate the elastoplastic stress and strain fields which ensure the mechanical equilibrium between a diffusively growing phase and its parent phase. Previous works (Barbe et al., 2007; Hoang et al., 2007; Barbe et al., 2008) have provided analysis of several effects of modelling parameters: boundary conditions, hardening laws, mesh size, nuclei density, etc. A methodology based on ensemble averaging has been developed, which enables determining effective properties of a representative volume element in small FE domains of computation without any mesh size effect. This work presents an extension of the modelling to the case of nucleation at preferential sites of austenite (quadruple points), which is proved to provide a spatial distribution significantly different from the uniform random case. The original resulting analysis shows that the spatial distribution of the product phase nuclei may influence TRIP. This means that if that distribution is modified prior to the transformation, which is expected to be the case when there is a pre-hardening which might generate new preferential nucleation sites, the development of TRIP can be affected. Clearly, the global transformation kinetics, which is often the only piece of information retained in a classical TRIP test, is not sufficient; the ‘internal’ parameters of the transformation such as spatial distribution of nuclei, kinetics of nucleation and kinetics of growth should be considered to improve modelling.

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