NUMERICAL DETERMINATION OF DIFFUSIONAL TRANSFORMATION INDUCED PLASTICITY FROM COMPUTATIONS OF RANDOM MICROSTRUCTURES

F. Barbe, R. Quey, L. Taleb
LMR, INSA de Rouen, F-76801 Saint Etienne Du Rouvray, France

Summary This work presents a finite elements approach for the modeling of diffusional transformation induced plasticity in a macro-homogeneous volume containing randomly-positioned nucleates. Assuming ergodicity, the effective TRIP is determined through ensemble averages over sub-domains extracted randomly from the bulk material.

INTRODUCTION

Solid-solid phase transformations of metals under applied stress can lead to permanent strains of the medium being transformed. They occur even though the loading stress is well below the yield stresses of all constituents. For this reason this phenomenon is usually refered to as TRansformation Induced Plasticity and requires improvements of classical plasticity formulations for its modeling. This has been achieved with good quantitative agreements with experimental results by Leblond, Fischer, and, Taleb and Sidoroff [1–3]. Yet, as explained in [4], calling upon particular loading history of the transformed material, one may evidence the fact that predictions of TRIP from modeling and experimental measurements are opposite in signs: if, previously to the transformation, the material has been strained permanently in the direction of the tensile stress imposed during transformation and then unloaded, the modeled TRIP is tensile whereas the experimental TRIP is compressive. Numerical modeling can provide elements of comprehension of the mechanisms involved in the development of TRIP and thus contribute to improvements in theoretical modeling. With finite elements, one is able to simulate the transformation of a volume element by taking into account the main mechanical effects of phase transformation: a change in the volumic density and in the elastoplastic properties of the finite elements being transformed. By opposition to martensitic transformations where plates with particular orientations form quasi-instantaneously, the diffusional transformation considered in this study is supposed to be progressing from a nucleate with an isotropic continuous growth. The question as to how the computed TRIP may be affected by the spatial distribution of nucleates, the number of elements in the mesh, the number of nucleates in the mesh and other parameters has been addressed in a previous study [5] and is still in the process of completion; it is the object of the first part of this summary. Then we present a method to compute the effective TRIP in a macro-homogeneous volume with a given density of randomly positioned nucleates.

NUMERICAL MODELING AND RESULTS

Spherical transformation from a single nucleate

The direct computation of a volume representative of a macro-homogeneous medium –necessarily consisted of a large number of nucleates since they are positioned randomly– would require a mesh so huge that a single parallel computing can hardly be envisaged, as emphasized in [5]. This difficulty can be circumvented by considering that, rather than randomly positioned, the nucleates are distributed along a regular cubic array thus forming a periodic composite material made of austenite matrix and bainitic growing particulates. By further assuming that all nucleates appear at a same instant and grow at a same rate, one can restrict the volume of computation to a cubic cell with a single central nucleate. This is an approach proposed by Ganghoffer *et al* [6], which we have adopted to validate our computations with the finite element code ZeBuLoN and to make firsts comparisons to our experimental results about bainitic transformation [7]. The cubic region of study with a central nucleate is reduced to a eighth as the symmetries in geometry and loading allow it. The first element to be transformed is accordingly located at a corner of the cubic mesh. This latter is discretised into $n \times n \times n$ cubic 8-node elements. The diffusional transformation is proceeded through the transformation of the successive layers of elements surrounding the product phase region. Meanwhile, a constant tensile stress well below the yield stresses of austenite and bainite is imposed to one of the faces of the cube. Some results (voided symbols) are given in fig. 1a with TRIP as function of the volumic fraction of product phase. They are in good qualitative agreement with experimental results, but it is not so true when comparing quantitatively, and there remains a mesh size effect even for the largest sizes of mesh.

Ensemble averaging over random realisations

In order to respect the randomness in the positions of the nucleates, one can simply perform computations where there are several nucleation elements randomly positioned in the mesh, as has been presented in [6] with few computations. It has been demonstrated in [5] that such computations are strongly sensitive to mesh size, number of nucleates and, above all, spatial distribution of the nucleates. Fig. 1b illustrates this last point: 100 TRIP curves obtained from microstructures differing only in the positions of the nucleates (number of nucleates is fixed to 4) have been plotted. They display so large a dispersion that only by calling upon several tenth of realisations would one obtain an ensemble average over individual curves that is unsensitive to the number of

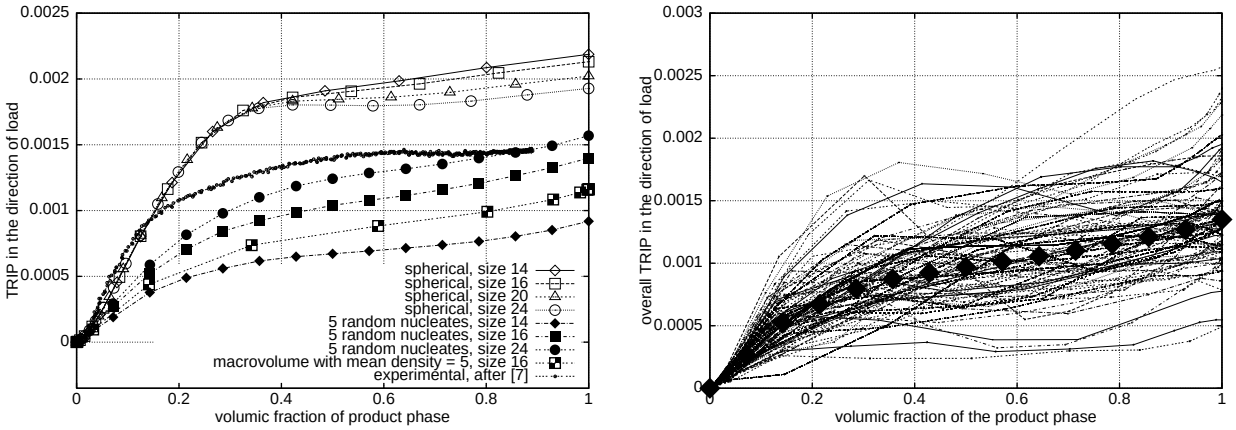

Figure 1: (a) TRIP obtained in different configurations of computations and experimentally. (b) TRIP computed in 100 microstructures with 4 randomly-positioned nucleates and the corresponding ensemble average result (◇)

realisations. It is further noticed on fig. 1a that the response computed by ensemble averaging (symbols filled in black) is dependent on the mesh size and, as shown in [5], on the number of nucleates: *(i)* the bigger the mesh the larger the TRIP, *(ii)* the larger the number of nucleates, the smaller the TRIP. Fortunately, the experimental curve is bounded by the responses provided by the computations on cells with single central nucleates (upper) and the responses determined by ensemble averaging (lower). Moreover, the bigger the mesh, the narrower the bounds. These considerations confirm that mesh size should be as large as possible and that, dealing with random distribution of nucleates, one gets a better quantitative agreement with experimental results. The slight increase in TRIP observed at the end of a transformation with random nucleates is partly due to the fact that, as compared to single nucleate cells, the probability of an austenitic element to be surrounded by bainite is much more important. Bainite having the highest yield stress, it can hold elastic stresses that would strain austenite plastically, all the more if austenite is embedded in bainite.

With the aim to perform random computations on a realistic macro-homogeneous medium, we have taken into account the fact that a sub-domain extracted randomly from the bulk material contains a number of nucleates that might vary with the position of the sub-domain. As nucleates positions are defined by a Poisson process, the probability of finding such or such number of nucleates in a sub-domain with a given size is known. The resulting set of probabilities (of finding 0 nucleate, 1, 2...) corresponds to the volumic fractions of all types of sub-domains encountered in the macro-volume. The effective response of the macro-volume is then obtained through an ensemble average over the responses in all types of sub-domain, balanced by their respective volumic fraction. The possibility for a sub-domain to be transformed partly or completely with the product phase growing from an external nucleate has also been implemented. An example of the results provided by the complete method is given in fig. 1a (symbol: half filled square): about 800 sub-domains of size $16 \times 16 \times 16$ have been extracted randomly from a quasi-infinite macro-volume; the density evolves from 0 to 7 nucleates per sub-domain and has a mean value equal to 5. This leads to an amount of TRIP significantly inferior to the one obtained with sub-domains of the same size containing strictly 5 nucleates (symbol: filled square), a difference that indicates that the full character of position-randomness in the macro-volume should be respected.

CONCLUSION

A classic method of the mechanics of disordered media have been adapted for problems of diffusional transformation. It is based on FE computations over meshes representing microstructures with nucleates varying randomly in their position and number. The effective TRIP is the result of a ensemble averaging balanced by the probabilities of finding such or such number of nucleates in a microstructure. Forthcoming improvements concern the optimisation of the number of computations required to get a result within a given interval of confidence.

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