COMPUTER SIMULATION OF INHOMOGENEOUS STORED ENERGY AND RECRYSTALLIZATION BY FINITE ELEMENT METHOD AND CELLULAR AUTOMATA

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Abstract *Microstructural evolution during recrystallization is a function of the stored energy of cold work. Existent analytical models normally assume that this free energy is uniformly distributed throughout the deformed matrix. However, in practice one observes that plastic deformation results in an inhomogeneous distribution of stored energy. This may significantly affect recrystallization kinetics. In this work, the distribution of stored energy was simulated by the finite element method (FEM). Taking these FEM results as our starting point, recrystallization was then simulated using cellular automata (CA). Using CA it was possible to study the effect of spatially inhomogeneous distribution of stored energy on overall recrystallization kinetics and microstructural evolution.*

Keywords*: Recrystallization, Cellular Automata, Finite Element Method, phase transformations.*

1. INTRODUCTION

Nucleation and growth solid state transformations are often modeled with the help of formal kinetics. In this methodology, nucleation and growth are regarded as purely "operational" concepts meaning that no assumption is made regarding their mechanism but only their geometrical and kinematical characteristics. Recrystallization kinetics in particular has been mainly analyzed with the help of formal kinetics methodology. The basis of formal kinetic modeling is the early work of Johnson-Mehl, Avrami and Kolmogorov (JMAK), (1939, 1940, 1941), which used only a single microstructural descriptor, the volume fraction of the transformed phase, V_V. JMAK's work was subsequently extended by DeHoff (1986), who proposed the use of an additional microstructural descriptor, S_V, and the associated concept of microstructural path. Vandermeer (1991, 1992, 2001) and coworkers extended DeHoff's microstructural path concept and crystallized it in an all round theoretical treatment covering variable nucleation and growth rates as well as non-spherical regions.

Nevertheless, even general analytical treatments have significant limitations owing to unavoidable simplifying assumptions. For instance, JMAK theory assumes that nuclei are randomly located in space. However, when one considers, for example, austenite to ferrite transformation, ferrite nucleates at grain boundaries. Another example is recrystallization, where the deformed state is, as a rule, highly heterogeneous casting some doubt on the assumption that nuclei are randomly located in space. Relaxing this and other assumptions may lead to situations that may require complex analytical methods when such an analytical approach is possible at all. In this regard, computer simulation of microstructural evolution can be an invaluable tool since it can simulate situations beyond analytical treatment. Compared to other simulation methods, cellular automata is a convenient choice for phase transformations in general and recrystallization in particular.

One situation that may occur during deformation is the development of deformation gradients, for example, during compression. Therefore, although nominally the specimen has undergone an average deformation the microstructure is not uniform and possesses deformation gradients that will influence subsequent recrystallization. In this work we use Finite Element Method (FEM) to simulate the development of deformation gradients generated during compression of a AA1100 Al alloy. Taking the FEM results as the starting point the specimen was then 'recrystallized' using cellular automata simulation (CA). In this paper we investigated only the effect of the deformation gradient of the velocity of transforming regions and assumed that nuclei were still randomly located. This work follows the Assis (2006) methodology to simulate strain and subsequent recrystallization by CAFE tool, (CA plus FEM).

2. SIMULATION

2.1 FEM SIMULATION

Firstly the plastic strain of the material was simulated by Finite Element Method in a quasi-static mode. The commercial program ANSYS 8.1 was used. The simulation of the Al 1100 cube compression was carried out assuming room temperature and isothermal conditions. Heating owing to friction between specimen and die was neglected.

The FEM model is schematically shown in Fig. 1. The specimen was a 40 x 40 x 40 mm cube. The specimen mesh consisted in 4096 solid elements of ANSYS type 'SOLID 45'. For the stress strain behavior of the Al-alloy Nagasekhar et al equation was used:

$$\sigma = 173.79\varepsilon^{0.304} \tag{1}$$

where σ and ε are the von Mises effective stress in MPa and plastic strain, respectively.

The dies (top and bottom) consisted of two rigid elastic blocks of an H 13 tool-steel with the Young modulus, *E*, and the Poisson's ratio, ν, equal to 200,000 MPa and 0.3, respectively. The mesh of each die consisted in 12,288 'SOLID 45' elements. All the degrees of freedom (DOFs) of the bottom die were restricted and in relation of the top die, only displacements in the global *y* direction downwards in Fig. 1, were allowed.

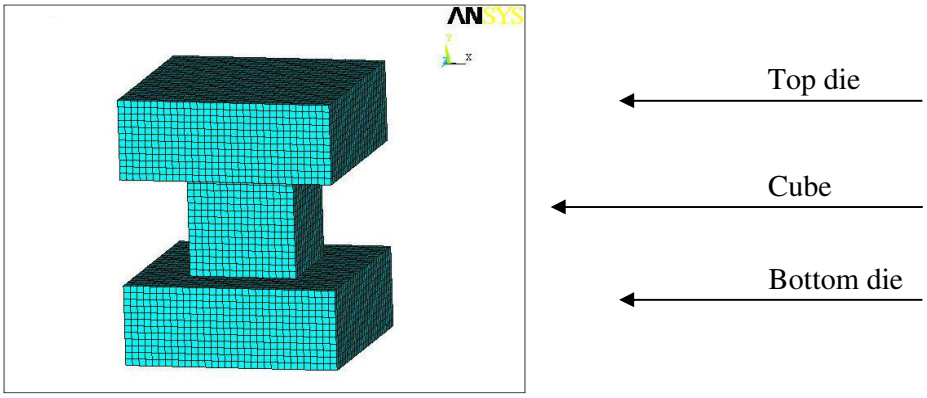

Figure 1. FEM modeling developed to simulate the compression of an Al 1100 cube

Constant increments of ram compressive displacements on the upper region of the top die were applied. The increments size was 0.25 and the simulation was carried out until the top die was displaced 18 mm, which is equivalent to a total strain of 45%. Full Newton-Raphson method with the automated line search convergence criteria and a sparse-type solver was employed with quadratic convergence. A friction coefficient value of 0.2 between specimen and die was used. To represent the friction behavior, the generalized Coulomb's law was used in the FEM models. In order to model the contact between specimen and die flexible-to-flexible elements were employed. The result of the FEM simulation is shown in Fig 2.

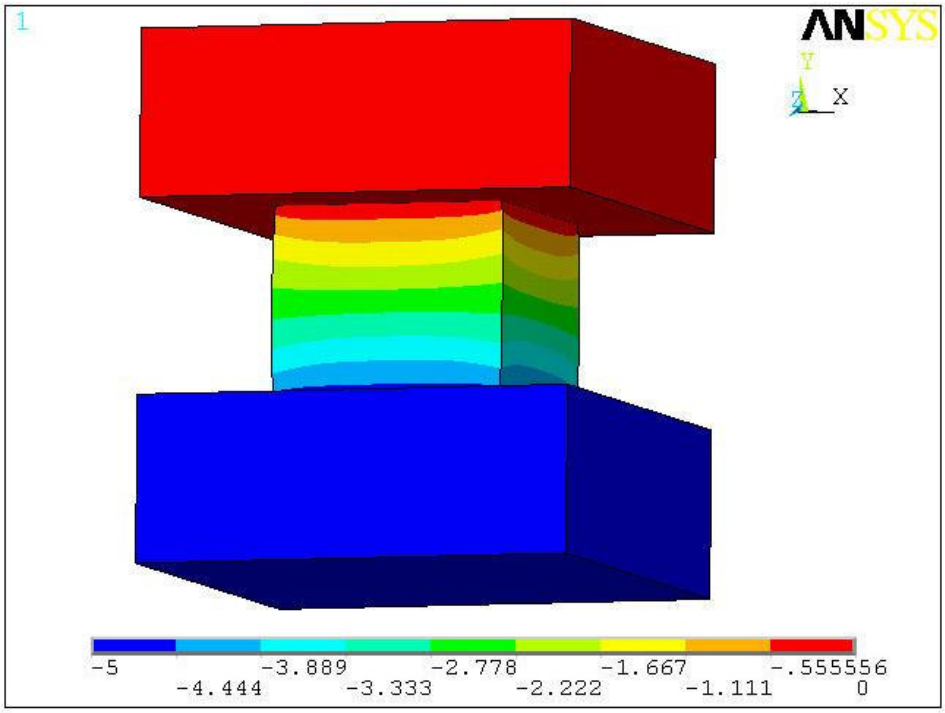

Figure 2.Distribution of the plastic strain in *y* direction during the simulation of the compression of an Al AA1100 alloy. The deformation ranges from 0 to 5.

2.2 C.A. SIMULATION

Cellular automata (CA) were employed as a computational tool to simulate recrystallization conform Hesselbarth and Göbel (1991) metodology. This implementation used the von Neumann neighborhood criterion in three dimensions. The matrix phase was represented by a cubic lattice with 304x304x304 cells together containing 4096 nuclei. Those input of data was been used in recent works sequence by Rios e*t all* (2005, 2006, 2007)

One cell edge was considered to have a unit length, and consequently each cell had unit volume. The units of all measured quantities reported here follow from this choice of unitary lattice parameter. The number of nuclei per unit of volume, N_V, was kept constant and equal to 1/6859. The matrix number of cells and of nuclei were chosen for reasons described elsewhere Nucleation was site-saturated, so all nuclei appeared simultaneously at t=0 and were randomly located within the cubic matrix. Time is a discrete variable in CA, as it assumes integer values starting from t=0. One time unit corresponds to the interval between two consecutive matrix updates. All the desired quantities could be extracted from the simulated matrices. Further details for three-dimensional CA simulation can be found elsewhere.

The results of FEM simulation were introduced in this matrix only qualitatively. It was observed that the deformation resulting from compression ranged roughly from 0 to 5, see Fig. 2. From this observation we assigned five energy levels to the CA matrix, also ranging from 1 to 5. The CA matrix was then divided in five parallel 'slices' and to each slice a corresponding energy level ranging from 1 to 5 was assigned so that the matrix possessed an energy gradient. In order to be used as a reference, CA simulation was also carried out in homogeneous matrices with uniform energy levels equal to 1 and 3, which is the average level. The results of this simulation are used as a reference. The velocity was proportional to the energy level of a particular cell. The CA matrices are shown in Fig. 3.

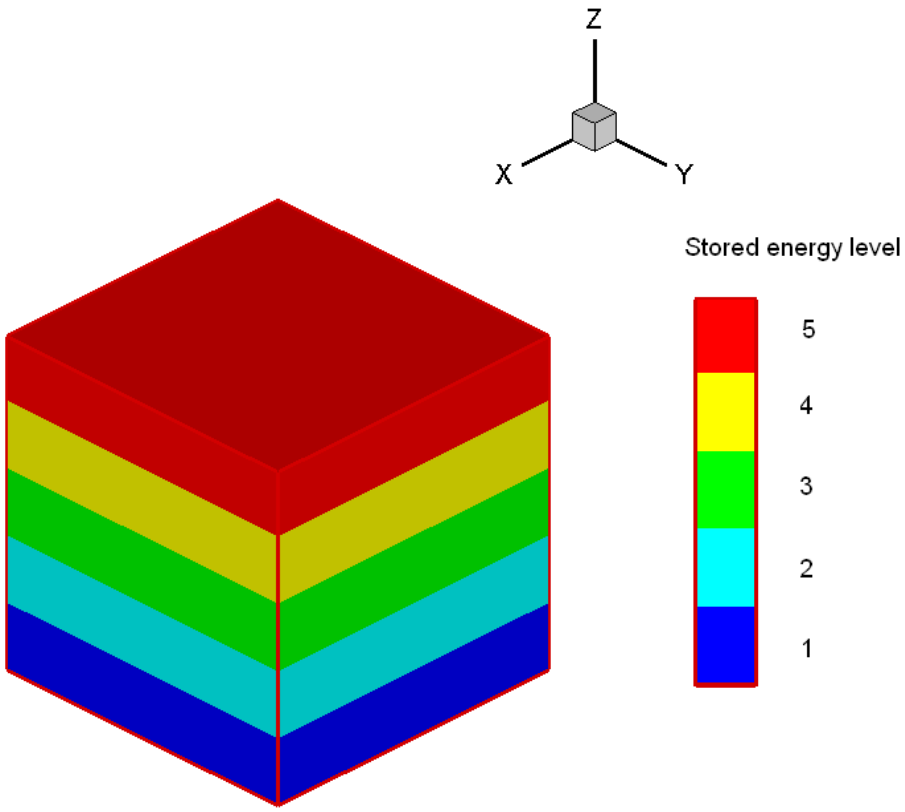

Figure 3 a. Representation of the matrix strained with strain gradient

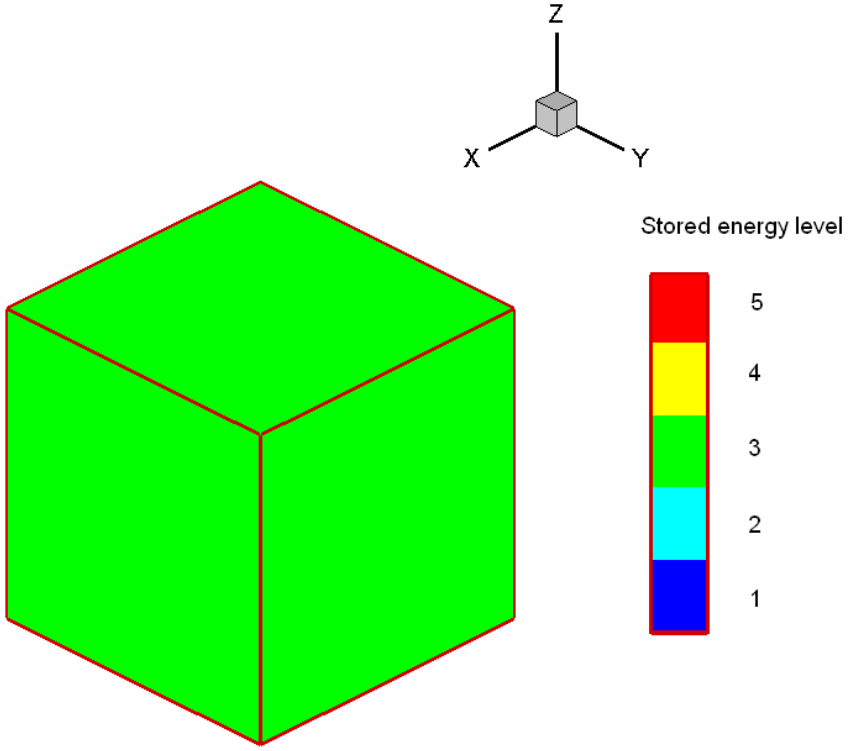

Figure 3 b. Representation of the matrix strained without strain gradient.

Figure (3a and 3b) – CA matrices used during simulation: a) heterogeneous matrix with the five energy levels and b) homogeneous matrix with energy level equal to 3. A matrix with an energy level equal to 1 was also used.

2.3 RESULTS AND DISCUSSION

The results of the simulation are shown in Figs. 4-8.

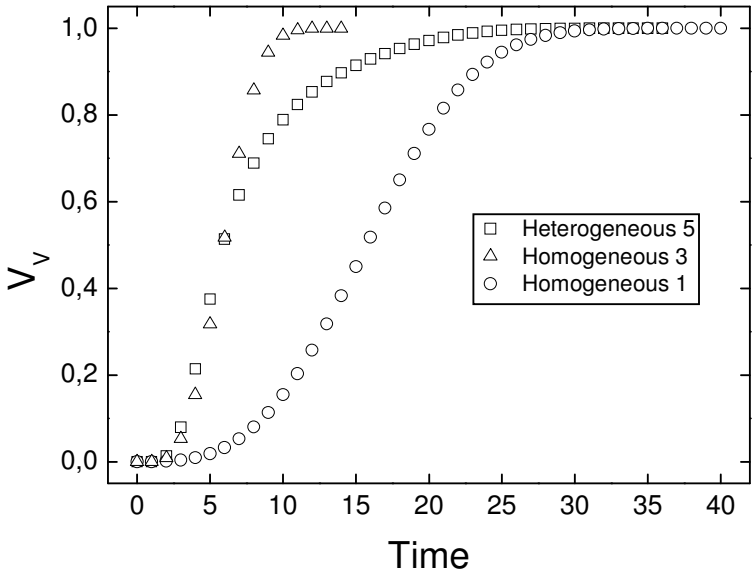

Figure 4. Volumetric fraction versus annealing time during computational simulation.

Fig. 4 – The transformation kinetics of homogeneous and heterogeneous matrices are compared in this figure. Homogeneous-3 and homogeneous-1 correspond to the matrices with a uniform distribution of energy used here: one with a stored energy level equal to 3, another with an energy level equal to 1. The transformation kinetics of the homogeneous matrix with energy level equal to 3 is initially close but still slightly slower than the kinetics of the heterogeneous matrix. But for a volume fraction transformed above about 0.5 the transformation kinetics of homogeneous matrix becomes significantly faster. By contrast, the transformation kinetics of the matrix with a low energy level, energy level 1, is always slower is than that of the heterogeneous matrix. However, towards the end of the transformation, the transformation kinetics of the heterogeneous matrix approaches that of the homogeneous matrix. This point is discussed further in the text.

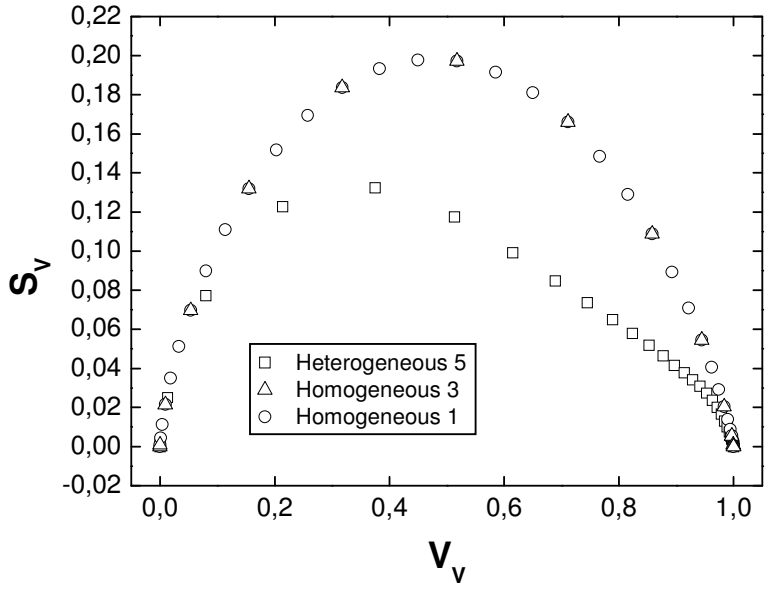

Figure 5. Surface fraction versus volumetric fraction during computational simulation.

Fig 5 is the micristructural path of the transformations representation, The difference between heterogeneous and homogeneous matrices is clear in this figure. The microstructural path, as theoretically predicted, is the same for both homogeneous matrices. By contrast, the microstructural path for the heterogeneous matrix is skewed.

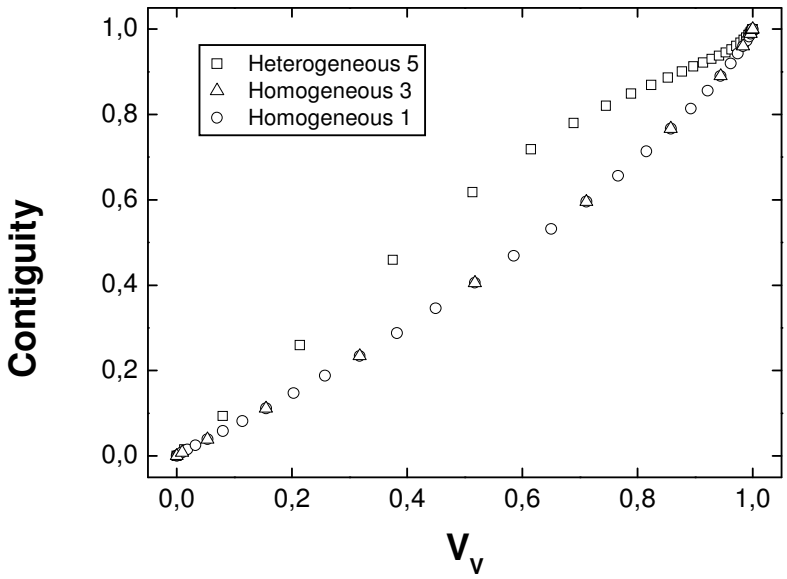

Figure 6. The contiguity, C_R, is plotted as function of volume fraction.

The contiguity is a parameter that reveals departures from randomness in the relative amounts of the interfacial area between transformed and untransformed regions, S_V, and of the interfacial area between transformed and transformed regions, S_{VR}. The contiguity is defined as:

$$C_R = S_{VR} / (S_V + S_{VR}) \quad (2)$$

The contiguity and also shows a clear difference between heterogeneous and homogeneous matrices. As theoretically predicted, it is the same for both homogeneous matrices. By contrast, it is significantly different for the heterogeneous matrices. This departure from randomness is a consequence of inhomogeneous growth in the heterogeneous matrix.

All the four figures above demonstrate quite convincingly the profound influence that a gradient of stored energy exerts on the transformation kinetics and on the resulting microstructure evolution. This is shown to be true even if nucleation was random, *i. e.*, nuclei were randomly located within the matrices. Of course an even stronger effect was to be expected if nuclei occurred preferentially at the highest energy regions.

The difference in transformation kinetics, see Fig. 4, stems from the fact that nuclei located in the highest energy regions grow faster because they may grow faster in those regions since the velocity is proportional to the stored energy. As a result, transformation is faster at the beginning but, as the highest energy regions are quickly consumed, the reaction slows down as it now must progress on the lower energy regions where the velocity is lower. This is clearly shown in Fig. 4 from the fact that towards the end of the transformation the transformation kinetics of the heterogeneous matrix approaches that of the homogeneous matrix with the low level of stored energy.

The influence on microstructural evolution is better seen in Figs. 5 and 6. Both the microstructural path and the contiguity show a significant difference between the microstructural evolution for heterogeneous and homogeneous matrices. It can be theoretically shown that both the microstructural path and the contiguity must be the same for the homogeneous matrices with random site-saturated nucleation. This difference in microstructural evolution reflects a departure from randomness of transformation of the heterogeneous matrix even though nucleation was random. This randomness was introduced by directionality of growth resulting from the stored energy gradient and by the inhomogeneous distribution of growth velocity. The contiguity curve of the heterogeneous matrix lies above the curve for the homogeneous matrix. If the velocity were constant this would mean that the nuclei were clustered. In this case, however, the nuclei are randomly located. Still one might say that growth is 'clustered' in the sense that the velocity within each region with a given stored energy is roughly the same but the velocity changes from region to region.

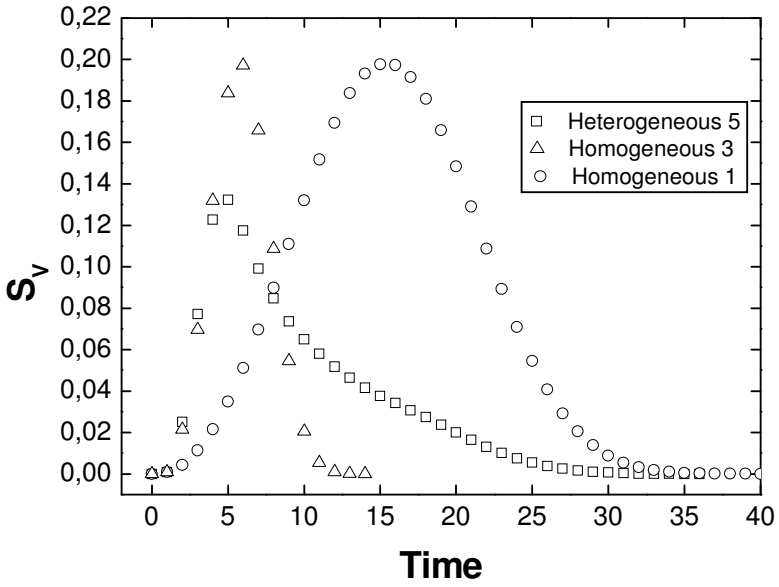

Figure 7. Surface fraction versus annealing time during computational simulation.

In the fig. 7 is shown surface fraction against annealing time, in this picture there are two curves with homogeneous energy distribution, and one with energy gradient.

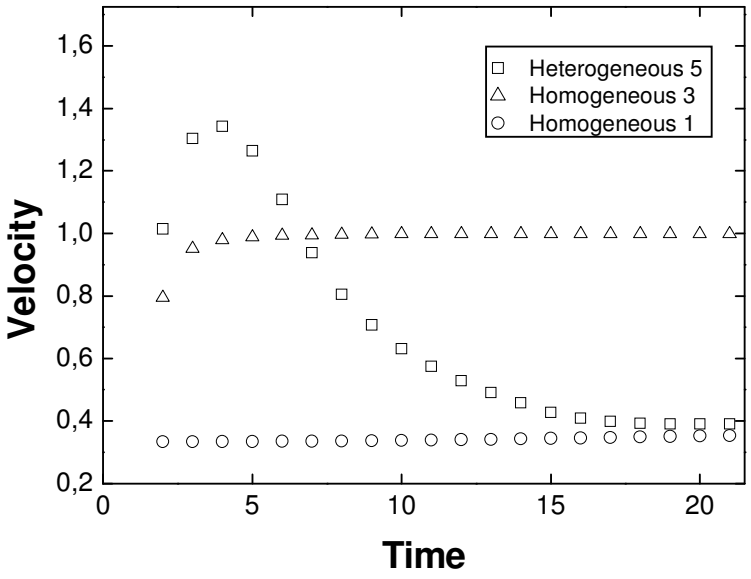

Figure 8. Interface velocity versus annealing time during computational simulation.

By fig. 8 it observes that when the energy is allocated homogeneously, the interface velocity permanence constant in time function. In all simulations the recover effect is discarded.

2.4 CONCLUSIONS

The present results show a significant effect of a gradient of stored energy both on the transformation kinetics and on the microstructural evolution.

The effect observed here was a purely growth effect since the nucleation was kept random.

The interface velocity really decrease when exist strain gradient on the matrix.

The two methods are very good tools for study qualitatively the strain and annealing in metallic materials.

3. ACKNOWLEDGEMENTS

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5. RESPONSIBILITY NOTICE

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