Materials Science Forum Vols. 738-739 (2013) pp 137-142
Online available since 2013/Jan/25 at www.scientific.net
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doi:10.4028/www.scientific.net/MSF.738-739.137

Dynamical behavior of martensite-austenite transitions: simulations and experiments

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Keywords: Solid-solid phase transitions, Martensitic transformations, Numerical simulations, Atomistic model, Cu-Zn-Al alloys, Mechanical experiments, Heating rate, Variant configuration.

Abstract. The dynamical behavior of the reverse martensitic transformation has been numerically simulated with an atomistic model and compared with experiments in Cu-Zn-Al alloys. Starting from different configurations of the martensitic variants (varying mainly their mean size), the transformation to austenite was studied as a function of the heating speed. Both, experimental and numerical results show that at low velocities there is no dependence of the transition temperatures, whereas at higher speeds they gradually increase. Simulations allow us to have an insight of the underlying processes during the transition to austenite. They also show that a heating speed independent transition can only be obtained when a microstructure of very small variants is present.

Introduction

Martensitic transformations (MT) are solid-solid phase transitions between a high symmetry phase called austenite and a low symmetry one called martensite. Being first order and diffusionless, these transformations play a prominent role in shape memory alloys, because the concomitant elementary processes govern the main effects that these materials present [1]. Such materials are mainly alloys of metallic elements, but there are also ceramic materials having this property [2]. In all these systems, the transformation usually occurs due to entropic effects as the temperature is changed. There is an effective dependence of the parameters of the system on temperature in spite of the fact that thermal diffusion is negligible during the transformation. Several materials showing MT display remarkable phenomena as shape memory and superelasticity, among others, which endows them with many practical applications as well as very interesting theoretical aspects [2].

Central to the phenomenology of martensites is the fact that from a single crystal of austenite, only few different martensitic orientations (variants) can be obtained. They can be thought as arising from different (symmetry related) distortions of the original structure when the martensite is formed. The self-accommodating character of the distribution of variants cannot avoid the generation of elastic strain energy due to the change of shape. Therefore, it can be thought that the phase equilibrium could be influenced by the change in the intervariant interface configurations. As far as we know, no systematic studies were done in order to understand both, the effect of the density of variants and the heating speed, on the transformation characteristics. This will be studied in the present paper.

Theoretical Model

We use a two-dimensional (2D) two body classical interaction potential that has a repulsive core at short distances and an attractive tail at long distances [3]. This potential is qualitatively similar to the standard Lennard Jones (LJ) one, but slight modifications are included to allow the stabilization

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of structures other than the compact ones. This produced a MT in the system and several interesting effects associated to them have been analyzed [3, 4]. In particular, a triangular-rhombohedral (T-R) transition in two dimensions can be driven by changing a parameter A_0, which weighs the repulsive part of the LJ term in the total potential. We found a critical value $A_0^c = 0.067$ above which the minimum energy state corresponds to a triangular (T) structure. For $A_0 < A_0^c$, the stable phase has a rhombohedral (R) lattice. The fact that the symmetry group of T contains that of R allows us to define T as the austenite and R as the martensitic phase. Variants can be thought as originated in distortions of the austenite triangular structure along different (but crystallographically equivalent) directions when the martensite is formed. Only three variants are defined in this model, characterized by the elongated side of the triangle [3].

In order to numerically study the transformations in 2D, we solve the time dependence of the particle coordinates according to the Verlet scheme, with the inclusion of a local friction term proportional to the velocities, which efficiently handles the thermal energy generated during the transition. The results shown in this work correspond to systems of around 40000 particles with open boundary conditions (a finite simulation domain and freely moving boundaries). This means that, in the case of temperature-induced MT, the shape of the boundary is completely determined by the interaction among particles. On the other hand, in the stress induced case the particles belonging to two stripes at opposite boundaries are forced to move as if they were grasped to the grips of a tensile machine. The model just described is able to produce the MT either by lowering the temperature or by the application of a stress.

The protocol to model a temperature-induced MT (here interpreted in terms of a variation of the A_0 parameter) is as follows. We start from a single crystalline sample of rectangular shape in a triangular (austenitic) structure by allowing the relaxation of the configuration through the dynamical algorithm at a constant value of $A_0 = 0.085$. We then slowly decrease the parameter A_0 at a constant rate v_A (ΔA_0 per calculation step), until the T-R transformation is completed. In Fig. 1 we show configurations of the system for $A_0 = 0.045$, where the transformation to the martensitic state is completed, for two different values of v_A. It can be seen that the number and size of the martensitic variants are highly dependent on the speed of the transformation.

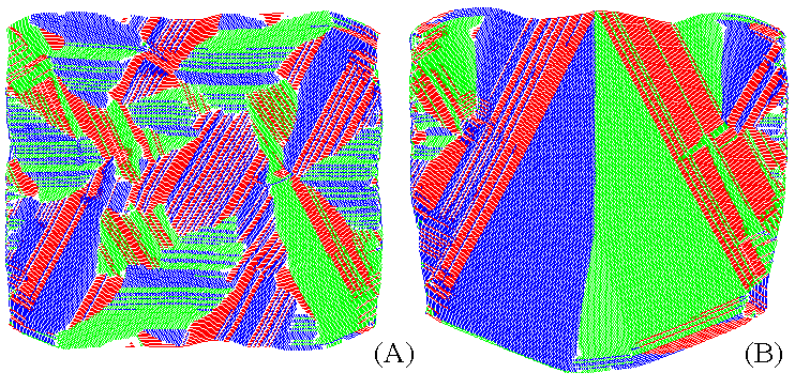

Figure 1: Snapshots of the final state of a temperature induced transformation when driven at two different speeds: (A) $v_A=10\times10^{-9}$ and (B) $v_A=1\times10^{-9}$. The three different colors indicate the three different martensitic variants. Particles in austenitic phase have no colors added.

It can be observed that slow transformations give rise to large variants and produce large shape deformations. On the other hand, a higher v_A drives a faster transformation which in turn produces a martensite with a highly twinned configuration of variants that easily accommodates, yielding a smaller change of shape.

In the present work we use these different microstructures as starting points to numerically study the dynamics of the reverse MT.

Experimental Method

The samples for electrical resistance (ER) measurements were prepared from austenitic single crystals of a Cu - 15.6 at%Zn - 16.2 at%Al alloy. A slab of around 1.2 x 1.3 x 40 mm^3 was cut. The standard four probe method was used, with a direct current of 30 mA. The four Cu wires were spot welded to the sample, as also the chromel-alumel thermocouple. The initial variant configurations were prepared as follows. The sample was cooled inside the ER equipment at two different speeds by controlling the liquid nitrogen level. This resulted in cooling speeds of 0.07 K/s and 0.3 K/s. A faster speed of 25 K/s was imposed by quenching the slab into liquid nitrogen and then placing the sample in the previously cooled ER equipment. The dynamics of the transformation to austenite was then studied as a function of these initial variant configurations and the heating velocities.

Additionally, a single martensitic variant specimen was obtained by inducing the transformation under stress. The composition of this sample was Cu - 13.6 at%Zn - 17.2 at%Al, in order to retain the martensitic phase at room temperature. The specimen was also cut from an austenitic single crystal, having a central part of 3 mm of diameter, a gauge length of 15 mm and thicker shoulders at the ends, appropriate to insert them into the grips of an Instron 1123 deformation machine. The strain was applied using a cross head speed of 0.2 mm/min, working at room temperature, to stress induce the martensite in the whole gauge length. This single variant configuration was then subjected to a set of heating speeds and the reverse transformation path was followed using dilatometry. The temperature was also measured with a thermocouple spot welded to the sample. The same sample was also tested in a polivariant state, obtained by quenching the austenitic phase into liquid nitrogen.

Numerical and Experimental Results and Discussion

We use the obtained martensites as starting point to study the dynamics of the transformation to austenite. This process can be quantified by plotting the evolution of the fraction of the system in martensite $\Phi_m = N_m / N$, being N_m the number of particles in the martensitic phase and N the total number of particles. We plot this quantity in Fig. 2A and 2B using the two initial configurations of Fig. 1 and three heating velocities. It can be observed that the reverse transformation from a multivariant martensite to austenite has no dependence with the heating speed for samples formed by numerous variants of small size (Fig. 2A). On the contrary, a clear dependence on the speed v_A is obtained for martensites composed of fewer and larger variants (Fig. 2B). For this variant configuration a constant transition path to austenite as in Fig. 2A is recovered for heating speeds below 1.

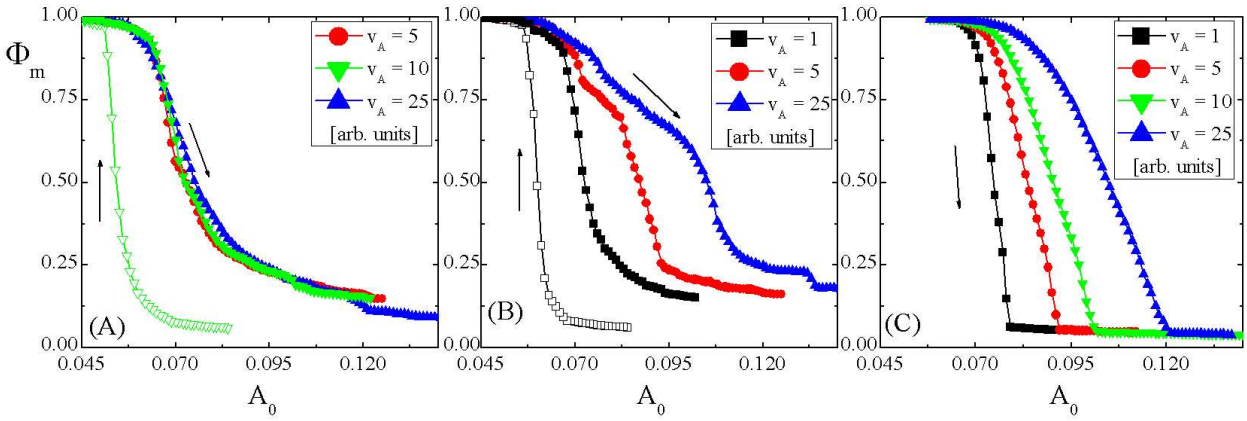

Figure 2: Evolution of Φ_m, the fraction of the system in martensite, as a function of A_0, the "temperature" parameter, for several rates v_A (speeds should be multiplied by a factor 10^{-9}). (A) From an initial variant configuration as in Fig. 1A. Full symbols correspond to the heating speeds indicated in the figure. Open symbols show the initial transformation path to martensite. (B) Similar to (A), but starting from Fig. 1B. (C) From a single-variant configuration obtained by a stress induced MT.

Based on these results, it seems interesting to eliminate the effect of variant boundaries on the dynamics of the transition to study separately the effect of the heating speed on reverse transformation. To do this we used a single-variant martensite obtained after a stress-induced transformation at $A_0 = 0.090$. As we discuss in previous works, this martensite is composed by only one variant that best fits the applied stress [3, 4]. By thermally inducing the transition from this martensite to austenite, we can isolate the effect of the heating speed on the reverse transformation. In Fig. 2C we plot the behavior of Φ_m for several heating speeds. It can be observed a shift of the transition to higher temperatures as the heating speed increases, as in the case of Fig. 2B. The shape of the curves suggests a more homogeneous transition path to the austenite when departing from the single-variant sample.

In the case of the experimental results, the fraction Φ_m was deduced from the ratio between the change of the measured property at each temperature and the total variation, after extracting the temperature dependence in the single phase regions. The results derived from the ER measurements are shown in Fig. 3A. The cooling speed has been change by a factor greater than 350, from which the variant configuration previous to the heating experiment was expected to have a considerable variation. The results indicate a behavior independent of the heating speed, in agreement with the simulations of Fig. 2A and/or the low velocities range in Fig. 2B. From these results it is not possible to determine whether a cooling speed of 0.07 K/s is slow enough to allow the generation of a microstructure with large variants. Therefore an increase of the experimentally affordable heating speed values was necessary.

This has been achieved in the dilatometric results of Figs. 3B and 3C, starting from polivariant and single-variant martensites, respectively. In both cases a clear dependence of the transition temperatures with the heating speed can be observed.

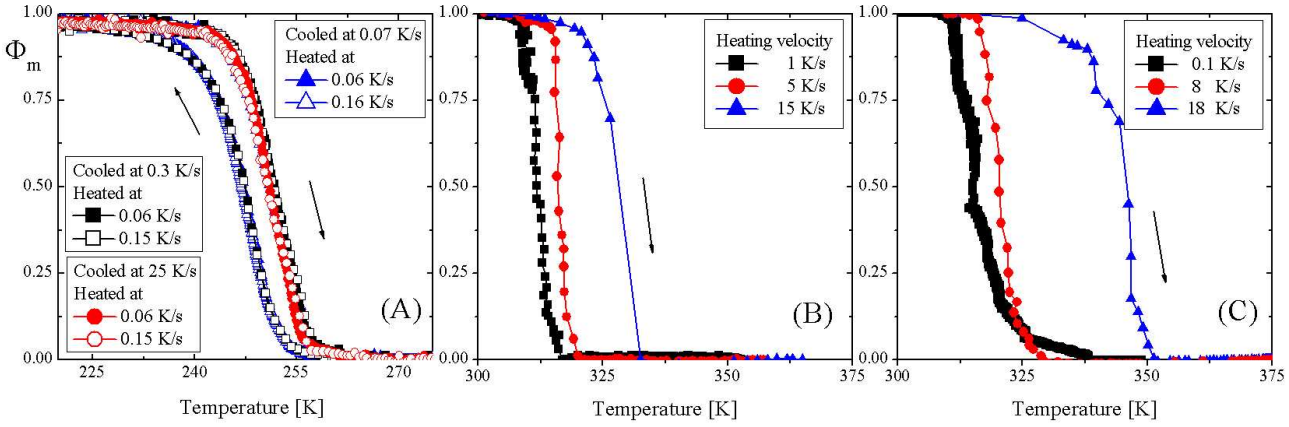

Figure 3: Evolution of Φ_m, the fraction of the system in martensite, as a function of the temperature. (A) ER measurements with a polivariant martensite at various cooling and heating rates. (B) Dilatometric measurements of a polivariant martensite at different heating rates. (C) Similar to (B) but starting from a single-variant martensite.

In order to analyze to what extent the variant configurations affect the transition, we compared the simulations and the experimental results by plotting the observed "temperature" shift as a function of the heating speeds. To this end we use the values for which half of the sample did already transform to austenite in the reverse MT branches of Figs. 2 and 3. In Fig. 4A we plot the shifts $\Delta T_{1/2}$, defined as $\Delta T_{1/2} = A_0(\Phi_m=0.5) - A_0^c$. On the other hand, in Fig. 4B the values are defined as $\Delta T_{1/2} = T(\Phi_m=0.5) - T_{min}$, with T_{min} the minimum value of $T(\Phi_m=0.5)$ for each set of measurements.

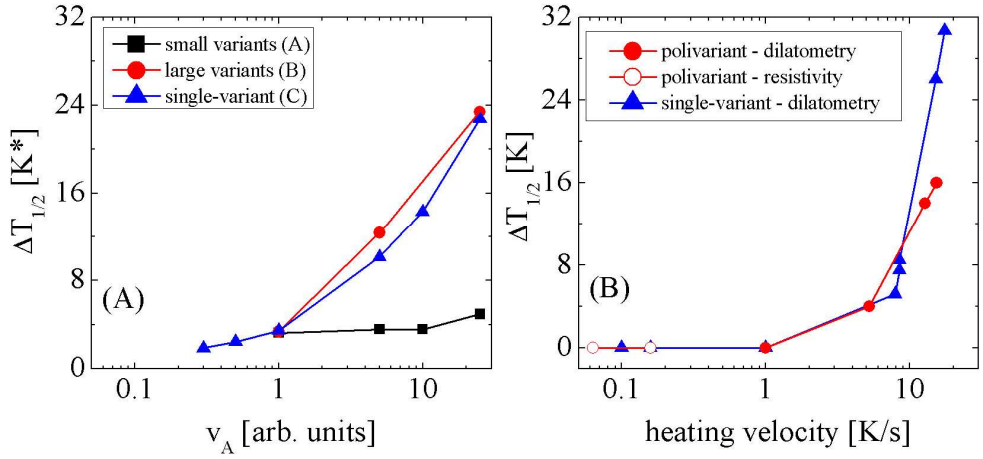

Figure 4: Shift of the transition as a function of the heating speed. (A) Numerical results for the three cases of Fig. 2. *The scale relationship between A_0 and the experimental temperature is obtained from Figs. 2 and 3, by equating the widths of the hysteresis cycles. (B) Experimental results, corresponding to the curves shown in Fig. 3.

It can be observed that the simulations and the experiments follow a similar trend, provided the case of the simulated small variants is omitted. The low velocities results seem to be independent of rate and configuration. The departure from this behavior becomes evident at higher speeds. The numerical results indicate that both, polivariant samples with large and few variants and single-variant ones have a similar behavior with velocity. This is in agreement with the experimental measurements, which present a temperature shift that is independent of the initial variant configuration. According to the simulations, a microstructure of small variants (as the one of Fig. 1A) is required to have a transition temperature almost independent of the heating rate. Apparently such variant configurations are not experimentally accessible, and the results of Fig. 3A would correspond to the ones in Fig. 2B for low heating velocities.

In order to understand the dependence with velocity at high heating speeds we analyzed the microstructure of the numerical sample during the transition. Simulations allowed us to directly observe the disappearance of the variants (not shown here). From the snapshots of the single-variant case we determined that, at low velocities, nucleation and growth of the austenite is rather inhomogeneous. The austenite starts from two opposite corners of the sample, producing a macroscopic deformation that, in turn, induces the quick disappearance of the martensite. At higher velocities, the martensitic phase is overheated and the austenite nucleated at higher temperatures grows more homogeneously. This implies a lower deformation of the sample that apparently accommodates better the remaining martensite. A similar behavior is observed for polivariant martensites consisting of large and few variants.

At present, we are working to quantify the degree of deformation as a function of the heating speed and its relationship with the way in which the variants disappear.

Summary

The dynamical behavior of the reverse martensitic transformation has been numerically simulated with an atomistic model and compared with experiments in Cu-Zn-Al alloys. For the calculations a model based on a classical isotropic two-body potential has been used. The samples were prepared from austenitic single crystals and cooled at different speeds or stressed to obtain several martensites differing in the size and shape of its variants. Then, the dynamics of the transformation to austenite was studied either numerically or experimentally by using ER and dilatometry. In this way, it was possible to study the effects of both, the size of the variants and the heating speed, on the reverse transformation characteristics.

Low velocities results are speed-independent, whereas high velocities produce an increase of the transition temperatures for both, simulations and experiments. Simulations have shown that, in order to have a fixed transition in the entire range of heating speeds it is necessary to have a martensitic microstructure consisting of very small variants. This seemed to be experimentally inaccessible for Cu-Zn-Al alloys. Simulations allowed us to have an insight of the underlying processes during the transition to austenite.

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European Symposium on Martensitic Transformations
10.4028/www.scientific.net/MSF.738-739

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10.4028/www.scientific.net/MSF.738-739.137