Journal of Alloys and Compounds, 211/212 (1994) 155–159
JALCOM 080

Numerical simulation of anelastic behaviour and microdeformation due to dislocations

J.F. Rojas
Departamento Física Aplicada I, EUITI, Universidad Pais Vasco, Plaza La Casilla 3, 48012 Bilbao (Spain)

J. San Juan
Departamento Física Materia Condensada, Facultad Ciencias, Universidad Pais Vasco, Apdo. 644, 48080 Bilbao (Spain)

M.L. Nó
Departamento Física Aplicada II, Facultad Ciencias, Universidad Pais Vasco, Apdo. 644, 48080 Bilbao (Spain)

Abstract

We introduce a general numerical simulation method that allows us to simulate different experimental conditions, getting the microcreep, elastic aftereffect and thermostimulated microdeformation curves. It also allows us to simulate the internal friction spectra *vs.* temperature in a similar way. The method is able to check the response of the material in these experimental tests as a function of the theoretical model in use and of the process activation parameters.

1. Introduction

The comparison between experimental results and theoretical predictions of the different models of dislocation mobility has been mainly qualitative to date, owing to the practical difficulty of producing quantitative predictions from these models. Because of the complexity an analytic solution to the problem is impossible; however, it is possible to do a study by numerical simulation on a computer.

The simulation studies carried out up to now have been particular developments applied to a concrete model of dislocation mobility and these studies have focused only on calculations of the internal friction (IF) [1–5], wasting the capabilities of other experimental techniques such as microcreep (MC), elastic aftereffect or microcreep recovery (MCR) and thermostimulated microdeformation (MD), collectively known as quasi-static techniques [6].

For this reason we introduce here a general methodology of numerical simulation whose main objective is to simulate the dislocation mobility process in order to calculate the results that will be obtained experimentally by all the above-mentioned quasi-static and dynamic techniques assuming the validity of a specific theoretical model. The method introduces all the dependences of the concrete model in a parametric way and in an independent and replaceable program module.

2. Numerical simulation

The calculation method was previously described [7] from the point of view of the computational technique and that is not the objective of this paper. Here we will just give a short description of the different parts of the simulation process, remarking on the most relevant physical aspects.

Firstly, we build up the energy diagram corresponding to a dislocation loop of length L submitted to internal stress σ_i and applied stress σ_a in the crystalline lattice of the material. It is in this program module that we introduce the physical model of dislocation mobility that we would like to use for the simulation process. In this way, the calculation methodology allows us to simulate processes in which the dislocation mobility is controlled by the Peierls barriers, or by intrinsic or extrinsic point defects etc.

In this paper we apply this method to simulate the dislocation mobility through the Peierls barriers of the crystal by the kink-pair-formation (KPF) process [8–10] within the constant-line-tension approach.

In this model, the energy diagram of the dislocation can be built up starting from three contributions:

$$E_T = E_p + E_\sigma + W_\sigma \quad (1)$$

E_p being the energy associated with the Peierls barriers, E_σ the energy corresponding to the line tension and W_σ the work of the stresses acting on the dislocation.

SSDI 0925-8388(93)00080-I

This is the kind of energy diagram that can be found in the literature [1–5]; it is probably not the most accurate, from a theoretical point of view, for use in the KPF process, as we will comment later. In the present paper, we use this model to allow us to compare our numerical results with the results of previously obtained simulations [1–5].

Once the energy diagram with the internal stresses σ_i is built up, the statistical distribution is obtained from the total number of dislocations on the different valleys of the energy diagram, which constitute the initial dislocation distribution, and this sets the origin of the deformation. If a stress σ_a is now applied, the new energy diagram can be calculated and the equation

$$\dot{n}_i = \Gamma_{i-1,i} n_{i-1} + \Gamma_{i+1,i} n_{i+1} - (\Gamma_{i,i-1} + \Gamma_{i,i+1}) n_i \qquad (2)$$

can be solved for each of the energy valleys [2, 4], where n_i represents the number of dislocations in the i valley and $\Gamma_{i,i+1}$ and $\Gamma_{i,i-1}$ the jump frequencies of the dislocations from the i valley to the adjacent valleys on the energy diagram. The jump frequencies can be calculated from the height of the barriers in the energy diagram and from the temperature T [7]. In this way, we let the dislocation distribution evolve during a precise time Δt, after which the deformation caused by the mean dislocation advance can be calculated. From this basic process, we can obtain the deformation produced by an applied stress σ_a during a period of time Δt at a temperature T.

The results obtained with the described simulation method will be presented for the special case of iron. The dislocation mobility in iron has been previously studied by MC, MD and IF (see ref. 11 for a review). The mobility of the non-screw dislocations due to the KPF process is responsible for the α relaxation at low temperatures (between 5 and 45 K). For this reason, the average values obtained experimentally for the α relaxation [11] were taken for our process.

In the case of the MC measurement, the energy diagram is built up by first taking account of the internal stresses, and the non-disturbed dislocation population in each energy valley of the diagram is obtained. A constant stress σ_a is then applied, and after calculating the new energy diagram the deformation ϵ_a at time intervals Δt is obtained to build up the curve $\epsilon = \epsilon(t)$. For the MCR simulation, after reaching the complete relaxation in the MC curve, the applied stress is suppressed and the energy diagram is calculated again. We obtain the deformation ϵ_a at time intervals Δt to build up the curve $\epsilon = \epsilon(t)$. Both processes happen at T = constant.

In Fig. 1 we show six MC curves obtained at different temperatures in a case in which we consider a dislocation length of 5000 Burgers vectors and an internal stress of 5×10^{-4} μ, μ being the shear modulus. The MCR curves corresponding to the previous MC curves after releasing the applied stress are shown in Fig. 2. In each case the MC curve was completely relaxed before releasing the stress in order to obtain the MCR curve at $\epsilon_0(\infty)$.

In the case of the MD measurements, first the initial energy diagram is built up in a similar way to before. A constant stress σ_a is then applied, and the new energy diagram is calculated. After this, the temperature is increased at a constant heating rate and the deformation ϵ_a is obtained at time intervals Δt to build up the curve $\epsilon = \epsilon(T)$. In Fig. 3 we show five MD curves corresponding to the same case as before but at different heating rates.

The process for obtaining the IF is more complex because the σ–ϵ cycle, whose area is proportional to the IF, has to be built up. This process requires the σ–ϵ cycle to be divided into stress increments $\Delta\sigma$. In each step of the cycle, the corresponding energy diagram must be calculated as well as the net movement of the dislocations during a period of time Δt that depends on the oscillation frequency and the number of steps into which the σ–ϵ cycle is divided [7]. This process is repeated until some convergence criterion is reached and the σ–ϵ cycle is closed. At this moment the cycle area can be calculated numerically and as a consequence the IF value can be obtained. All this process is carried out at constant temperature, so we should repeat it at increments ΔT to obtain the $\phi(T)$ spectrum point by point.

The IF measurements in Fig. 4 were simulated for frequencies of 0.01, 0.1, 1, 10 and 100 Hz with an oscillation amplitude of 10^{-6}, an internal stress $\sigma_i = 5 \times 10^{-5} \mu$ and a dislocation length $L = 3200b$. The IF spectra simulated at different frequencies show the temperature shift that we can expect from a thermally activated process, and will be discussed later.

Once the general method of simulation is described, it is necessary to remark that the energy diagrams and the simulation results obtained for different values of the internal stresses σ_i and dislocation lengths L are clearly different [7]. For this reason, in order to obtain simulation results comparable with the real experimental measurements, it is necessary to include line length and internal stress distributions. However, the simulation work carried out taking into account these distributions will be presented in another paper because of space considerations.

3. Discussion

The best way of checking the consistency of the simulation results obtained is to consider them as experimental results. If we apply the usual methods

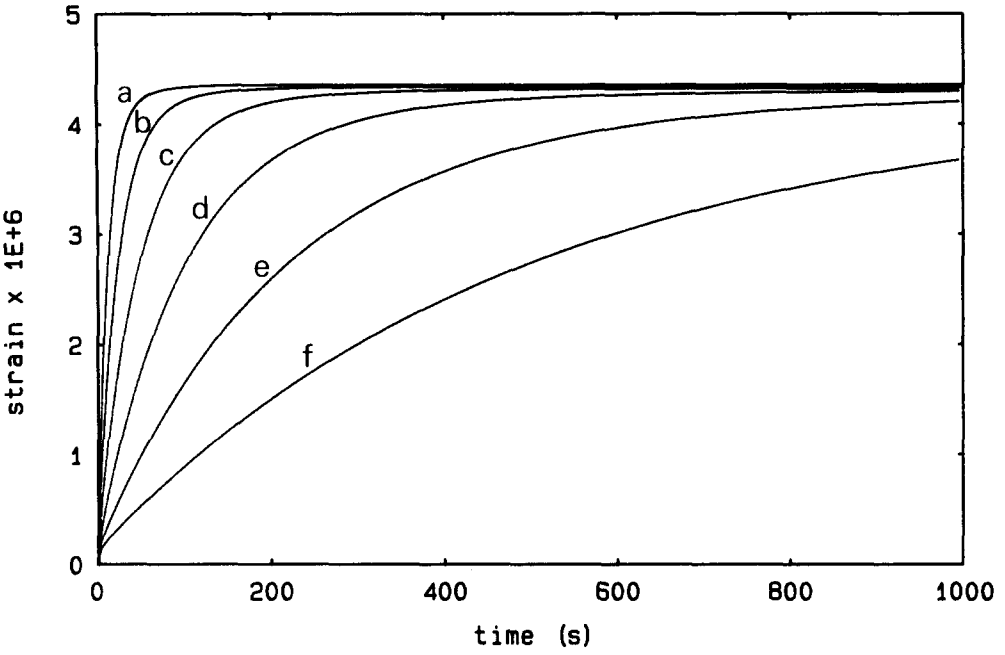

Fig. 1. MC simulated curves for a dislocation line of length $L = 5000b$, under stresses $\sigma_i = 5 \times 10^{-4}\mu$ and $\sigma_a = 10^{-4}\mu$, at six temperatures: curve a, 19 K; curve b, 18.5 K; curve c, 18 K; curve d, 17.5 K; curve e, 17 K; curve f, 16.5 K.

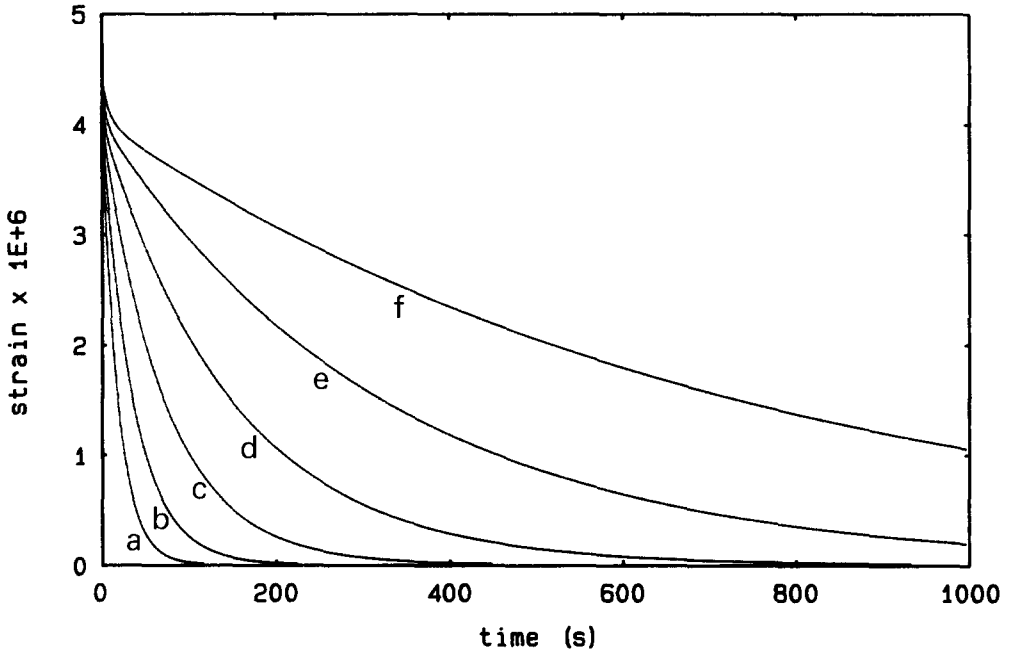

Fig. 2. MCR simulated curves for a dislocation line of length $L = 5000b$, under stresses $\sigma_i = 5 \times 10^{-4}\mu$ and $\sigma_a = 10^{-4}\mu$, at six temperatures: curve a, 19 K; curve b, 18.5 K; curve c, 18 K; curve d, 17.5 K; curve e, 17 K; curve f, 16.5 K.

for the determination of the activation parameters to our results we can verify whether the simulation method used is reliable. In order to do this, we plot the Arrhenius diagram corresponding to the maxima of the IF peaks of the simulated spectra at different frequencies for a simple case (with no distributions). The shifting in temperature of the peaks *vs.* frequency fits perfectly a straight line, giving an activation energy $E = 0.0435$ eV and a pre-exponential time $\tau_0 = 2 \times 10^{-10}$ s.

In the case of the MC and MCR curves, the results obtained can be fitted to the theoretical expressions with very high correlation. The characteristic relaxation time at each temperature can be obtained and represented in the Arrhenius diagram bearing in mind

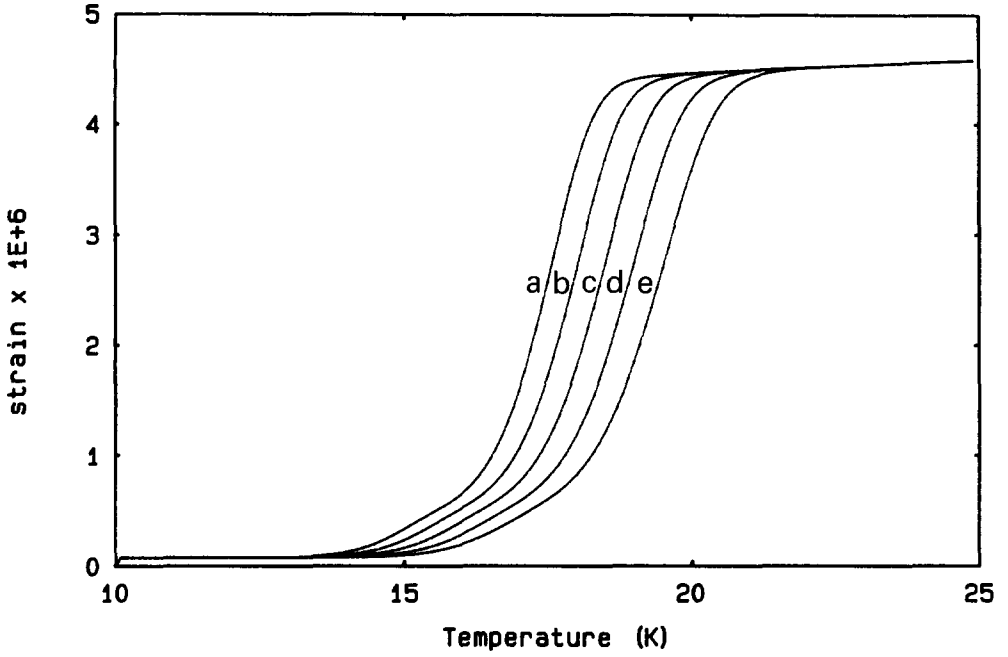

Fig. 3. Thermostimulated (MD) simulated curves for a dislocation line of length $L = 5000b$, under stresses $\sigma_i = 5 \times 10^{-4}\mu$ and $\sigma_a = 10^{-4}\mu$, at five heating rates: curve a, 0.5 K min^{-1}; curve b, 1 K min^{-1}; curve c, 2 K min^{-1}; curve d, 4 K min^{-1}; curve e, 8 K min^{-1}.

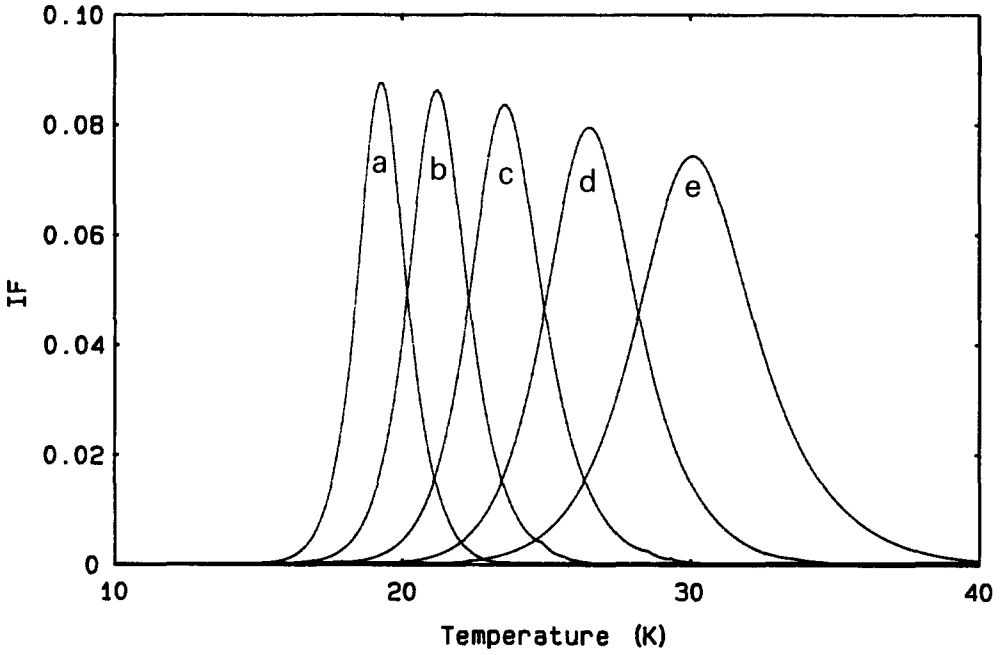

Fig. 4. IF simulated spectra for a dislocation line of length $L = 3200b$, under stresses $\sigma_i = 5 \times 10^{-5}\mu$ and $\sigma_a = 10^{-6}\mu$, at five frequencies: curve a, 0.01 Hz; curve b, 0.1 Hz; curve c, 1 Hz; curve d, 10 Hz; curve e, 100 Hz.

that $\omega\tau_\sigma = 1$. In this way, from the MC results we get an activation energy $E = 0.038$ eV and a pre-exponential factor $\tau_0 = 7.6 \times 10^{-10}$ s. In MCR, an activation energy $E = 0.040$ eV and a pre-exponential factor $\tau_0 = 3 \times 10^{-10}$ s are obtained. These values of the pre-exponential factor τ_0 of the relaxation time obtained by simulation are very close to that obtained experimentally (1.5×10^{-10}s) [11, 12] characteristic of the KPF process.

The activation energy obtained by MC simulation experiments is logically lower than that obtained by IF simulation experiments because of the contribution of the applied static stress work. The value of the activation

energy obtained by MCR is slightly lower than that obtained by IF because the dislocation movement takes place along a greater number of valleys during the MCR experiment. The mean energy barrier of the higher valleys is lower than that of the valleys close to the lowest minimum of the energy diagram, where the motion of the dislocations in an IF measurement takes place. In addition to this, the difference between the activation energies obtained and that introduced at the beginning of the program ($E = 0.045$ eV) is due to the curvature of the energy diagram around the lowest minimum position.

The MD curves show a peculiar behaviour just when they start rising like that observed in real experience [11]. The activation volume of the process can be obtained from the half-height temperature shift ΔT between two curves [14, 15]. In this way we get a value of $20.5b^3$ for the activation volume that is very close to the input value ($20b^3$).

In this first approximation one cannot expect the simulation results to fit the experimental real results, owing to the complex structure of the α relaxation in iron that shows three components [11, 12] linked to the KPF process plus another component α' at very low temperatures (between 5 and 15 K) linked to the geometric kink migration on the screw dislocations [11, 13]. A better approximation to the experimental results and a detailed analysis of the theoretical models requires the systematic introduction of the length and internal stress distributions already indicated.

Besides, we would like to remark that the profile used for the energy diagram may not be the best to simulate the KPF process as Benoit has commented [16]. In fact, it is not clear that the kink pair need overcome any barrier during the annihilation process. Instead we should consider that the relaxation of the kinks in a backward direction is probably controlled by the delayed motion of the kinks along the dislocation line. This aspect is being developed now and will be taken into account in a further refinement of our simulation process.

The simulation process developed leads to coherent results in good agreement with the experimentally obtained measurements as well as with the theoretical models of dislocation mobility, even using simple cases of calculation with no distributions at all. We can conclude that the method developed allows the simulation of the dislocation mobility under different experimental conditions in the anelastic range. The simulation results should be comparable with the experimental results if length of dislocation and internal stress distributions of the material are used.

Acknowledgments

We wish to thank Professor Benoit for his comment about the kink pair annihilation when releasing the applied stress.

This work has been carried out thanks to the financial support of the Comisión Interministerial de Ciencia y Tecnología in the framework of the Plan Nacional de Materiales (Project MAT 89-0554-C02-02).

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