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Procedure of identification of a constitutive law for homogeneous deformation of bulk metallic glasses

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► To cite this version:

Marc Bletry, P. Guyot, J.J. Blandin, J.L. Soubeyroux. Procedure of identification of a constitutive law for homogeneous deformation of bulk metallic glasses. European Congress and Exhibition on Advanced Materials and Processes Euromat 2007, Sep 2007, Nuremberg, Germany. hal-00196804

HAL Id: hal-00196804

<https://hal.science/hal-00196804>

Submitted on 31 May 2023

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1 Introduction

We propose a method to identify the parameters of a constitutive law based on the free volume model as proposed by Spaepen [Spa77] and taking into account the variation of the concentration of free volume with deformation, following the lines drawn by de Hey et al. [DHSVdB98].

2 Experiments

2.1 Elaboration and characterization

BMGs of composition $Zr_{52.5}Al_{10}Cu_{22}Ti_{2.5}Ni_{13}$ (G1) and $Zr_{52.5}Al_{10}Cu_{27}Ti_{2.5}Ni_8$ (G2) were produced. Characteristic temperatures of both glasses are:

glass	T_g (K)	T_X (K)	ΔT (K)
G1	659	761	102
G2	663	745	82

2.2 Compression tests

Compression tests at 683 K (strain-rate jumps and deformation-relaxation experiments).

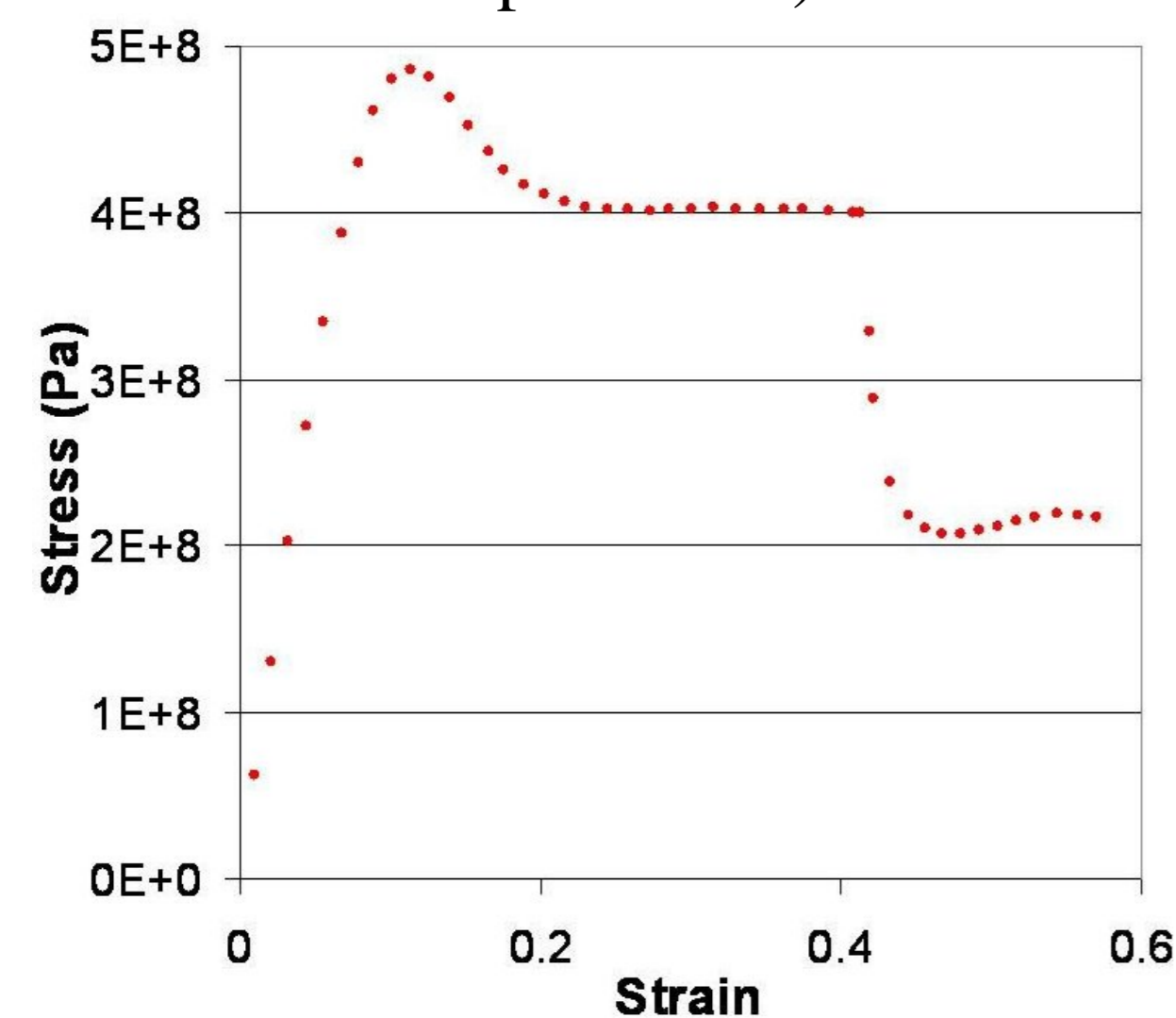


Figure 1: Strain-rate jump test at 683 K (from $2.5 \times 10^{-3} \text{ s}^{-1}$ to $5 \times 10^{-5} \text{ s}^{-1}$) on G2.

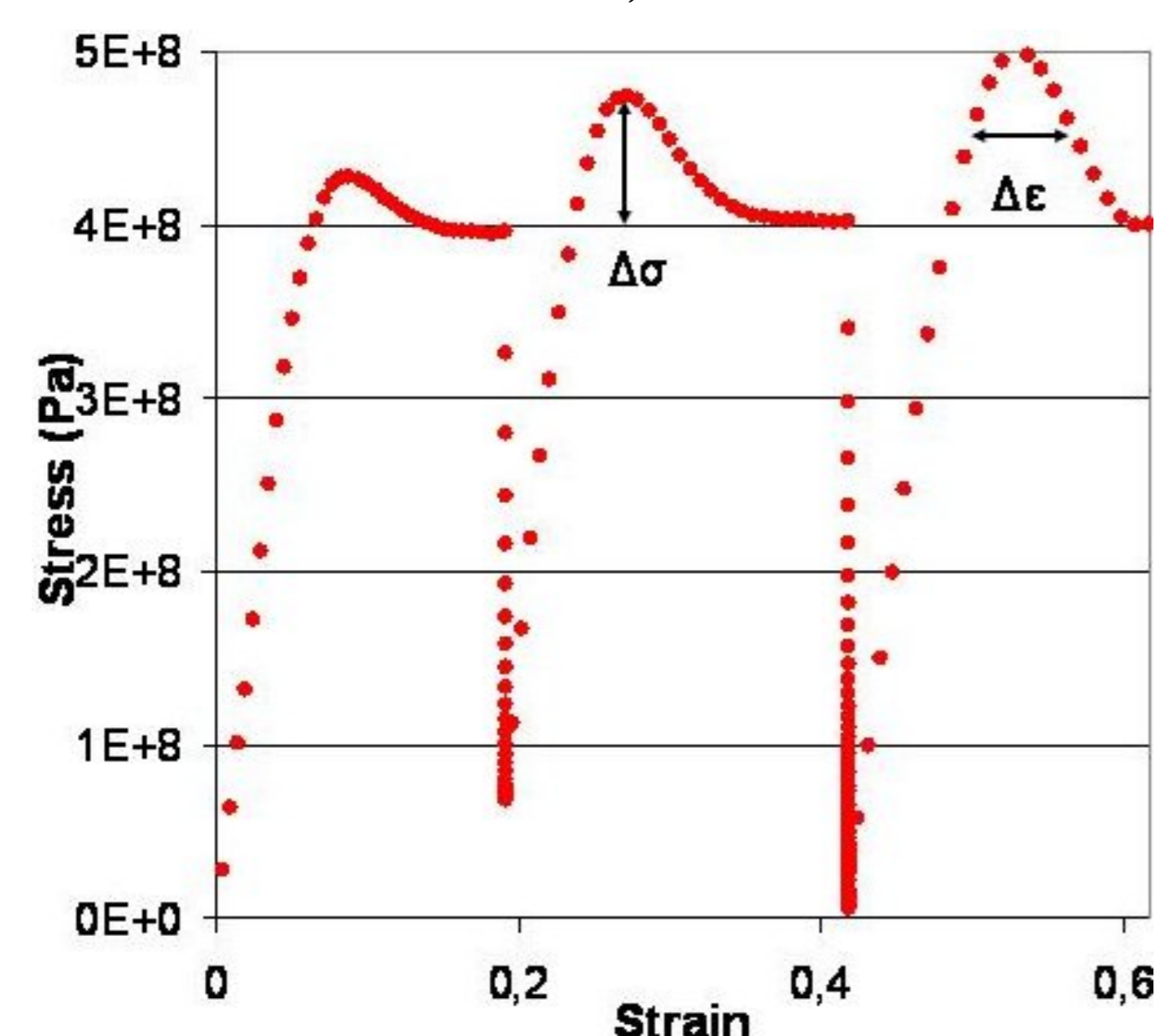


Figure 2: Deformation relaxation experiments at 683 K ($\dot{\epsilon} = 2.5 \times 10^{-3} \text{ s}^{-1}$) 1st relaxation: 57 s, 2nd: 1110 s, on glass G2. $\Delta\sigma$ and $\Delta\epsilon$ are the overshoots amplitudes.

3 Modeling the steady state

For uniaxial tests plastic strain-rate is (cf. [Spa77]):

$$\dot{\epsilon}_p = c_f \dot{\epsilon}_{0,c} \sinh\left(\frac{\sigma V}{2\sqrt{3}kT}\right) \quad (1)$$

c_f : flow defect concentration, $\dot{\epsilon}_{0,c}$: diffusion-like thermally-activated process, V : activation volume. Variation of c_f is (cf. [DHSVdB98]):

$$\dot{c}_f = a_x \dot{\epsilon}_p c_f \ln^2 c_f - k_r c_f (c_f - c_{f,eq}) \quad (2)$$

a_x : free volume creation coefficient, k_r : structural relaxation coefficient, $c_{f,eq}$: equilibrium flow defect concentration. At constant strain-rate, it comes [DHSVdB98]:

$$c_f^* = c_{f,eq} + \frac{a_x \dot{\epsilon}_p}{k_r} \ln^2 c_f^* \quad (3)$$

Combining equations (1) and (3) we get:

$$\frac{a_x}{k_r} = \frac{\dot{\epsilon}_{0,c} \sinh\left(\frac{\sigma V}{2\sqrt{3}kT}\right) - c_{f,eq}}{\dot{\epsilon}_p \ln^2\left(\frac{\dot{\epsilon}_{0,c} \sinh\left(\frac{\sigma V}{2\sqrt{3}kT}\right)}{\dot{\epsilon}_p}\right)} \quad (4)$$

$\dot{\epsilon}_{0,c}$ and a_x/k_r can be determined from compression tests, using experimental ($\dot{\epsilon}$, σ) couples from two plateaus (figure 1) forming a system of (slightly nonlinear) equations (eq. 4). It is impossible to determine V and/or $c_{f,eq}$ with this procedure (see [BGBS06],[BBG⁺]), but the dependency of $\dot{\epsilon}_{0,c}$ and a_x/k_r with them can be calculated (fig. 3).

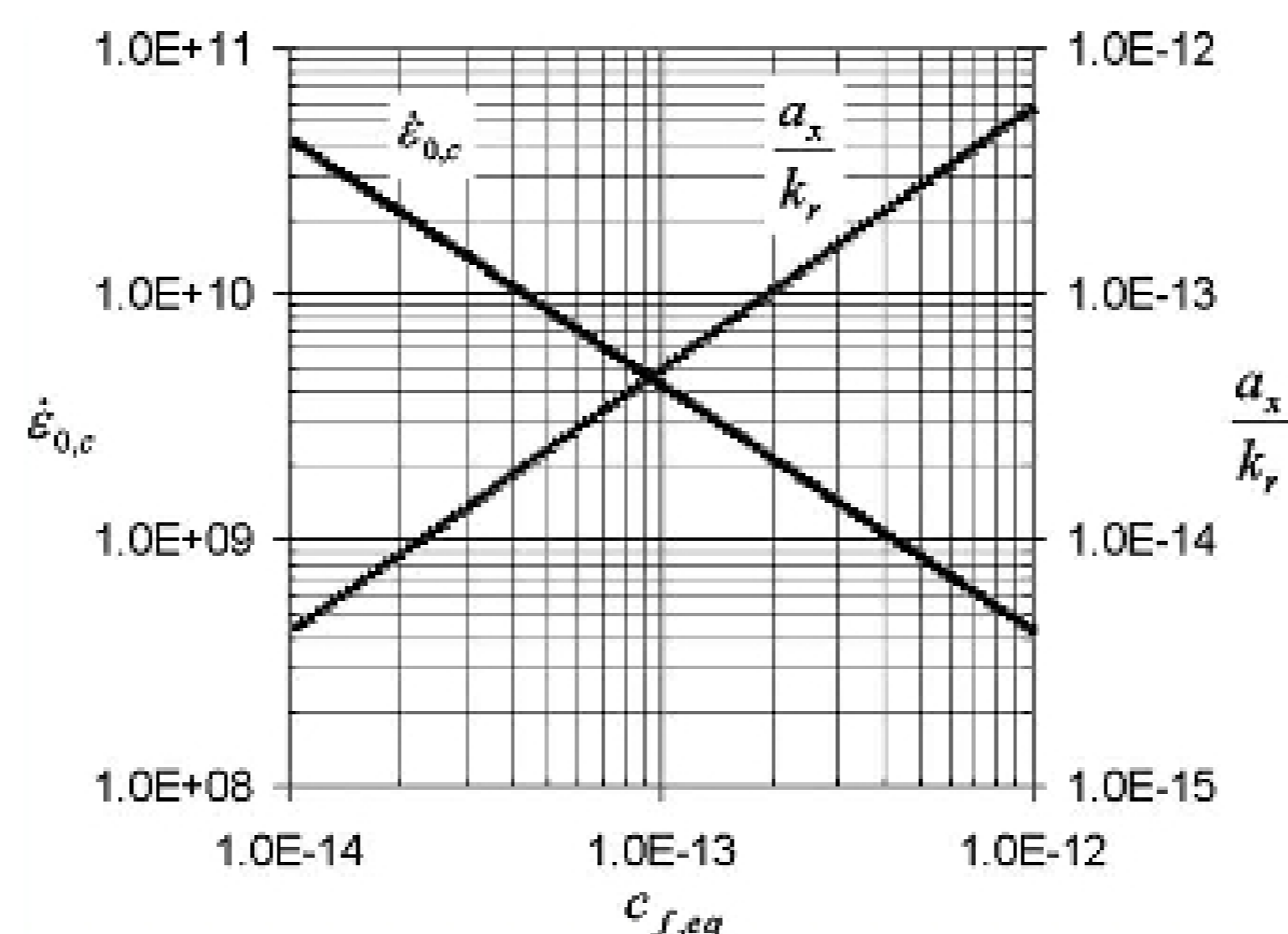


Figure 3: Dependence of a_x/k_r and $\dot{\epsilon}_{0,c}$ with $c_{f,eq}$ for a glass of composition G1 obtained from two experimental ($\dot{\epsilon}$, σ) couples at 683 K (see [BGBS06]): all these values of $c_{f,eq}$, a_x/k_r and $\dot{\epsilon}_{0,c}$ lead to the same rheology.

4 Modeling transient phenomena

4.1 Model

Most simple model to describe a whole stress strain curve:

$$\begin{cases} \dot{\epsilon}_T = \frac{\dot{\sigma}}{E} + c_f \dot{\epsilon}_{0,c} \sinh\left(\frac{\sigma V}{2\sqrt{3}kT}\right) \\ \dot{c}_f = a_x \dot{\epsilon}_p c_f \ln^2 c_f - k_r c_f (c_f - c_{f,eq}) \end{cases} \quad (5)$$

$\dot{\epsilon}_T$: total strain rate, $\dot{\sigma}/E$: elastic contribution. How can we determine the various parameters (i.e. a_x , k_r , V and $c_{f,eq}$)? Steady state analysis \Rightarrow how to get a_x/k_r and $\dot{\epsilon}_{0,c}$ with two plateaus. Then: parametric study of (5) with $\dot{\epsilon}_{0,c}$ known and constraint over a_x/k_r .

4.2 Parametric study

Young modulus E It is necessary to use $E \approx 10$ GPa (measured value at this temperature: ≈ 77 GPa), probably because of anelastic phenomena.

Kinetic parameters - a_x and k_r Fig. 4 shows that a_x and k_r control the overshoots amplitude: increasing a_x (and k_r : their ratio is set) \Rightarrow faster variation of c_f , \Rightarrow smaller overshoots and undershoots.

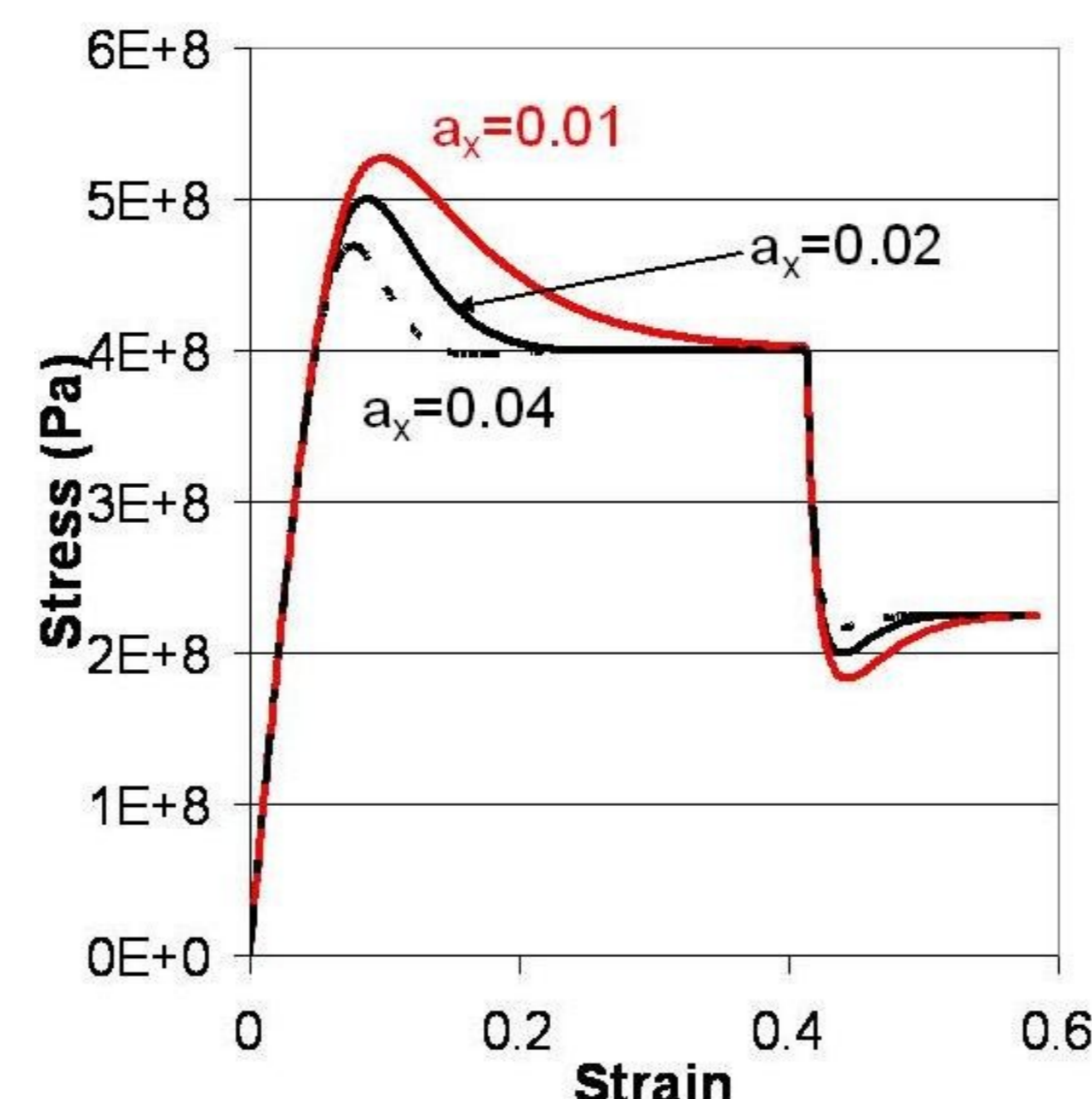


Figure 4: Parametric study of kinetic coefficients a_x and k_r , modeling the experiment presented figure 1.

For V and $c_{f,eq}$ given, it is possible to optimize a_x and k_r .

Activation volume - V To determine V the procedure is:

- various activation volumes V : steady state analysis \Rightarrow value of a_x/k_r and $\dot{\epsilon}_{0,c}$
- varying a_x and k_r \Rightarrow good value of $\Delta\sigma$
- good activation volume = the one with the good $\Delta\epsilon$

Figure 5 shows an application of this procedure.

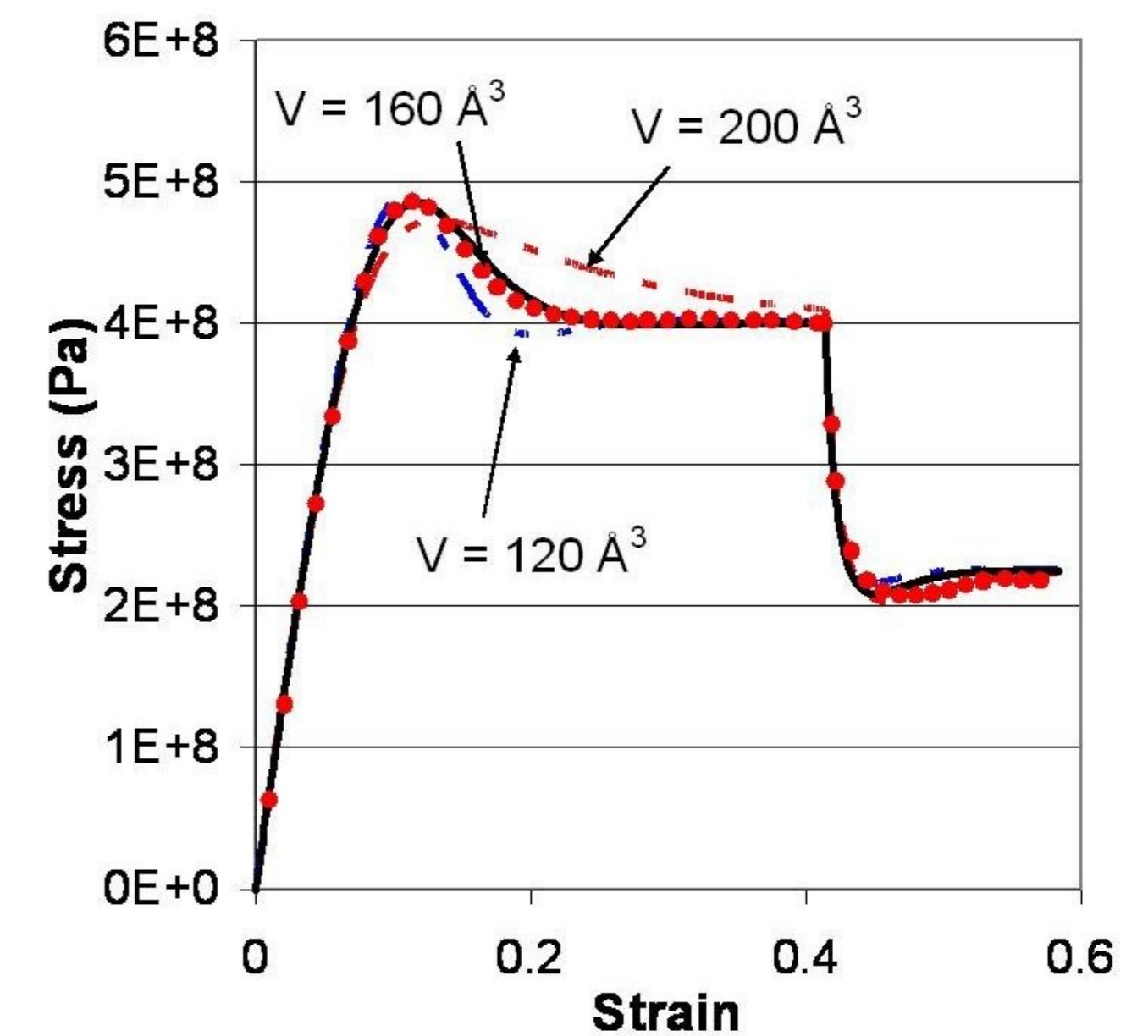


Figure 5: Parametric study of the activation volume (dots: experience of fig. 1). Each modeled curve uses the values of a_x and k_r that fits $\Delta\sigma$. Parameters of the black curve are given in the table below.

$c_{f,eq}$	E (GPa)	V (\AA^3)	$\dot{\epsilon}_{0,c}$	a_x	k_r (s^{-1})
10^{-12}	10	160	2.8×10^8	0.02	2.3×10^{10}

Equilibrium flow defect concentration - $c_{f,eq}$ It is impossible to determine $c_{f,eq}$, but the dependency of a_x and k_r with $c_{f,eq}$ that fits the same $\sigma(\epsilon)$ curve is shown in figure 6. V does not vary with $c_{f,eq}$.

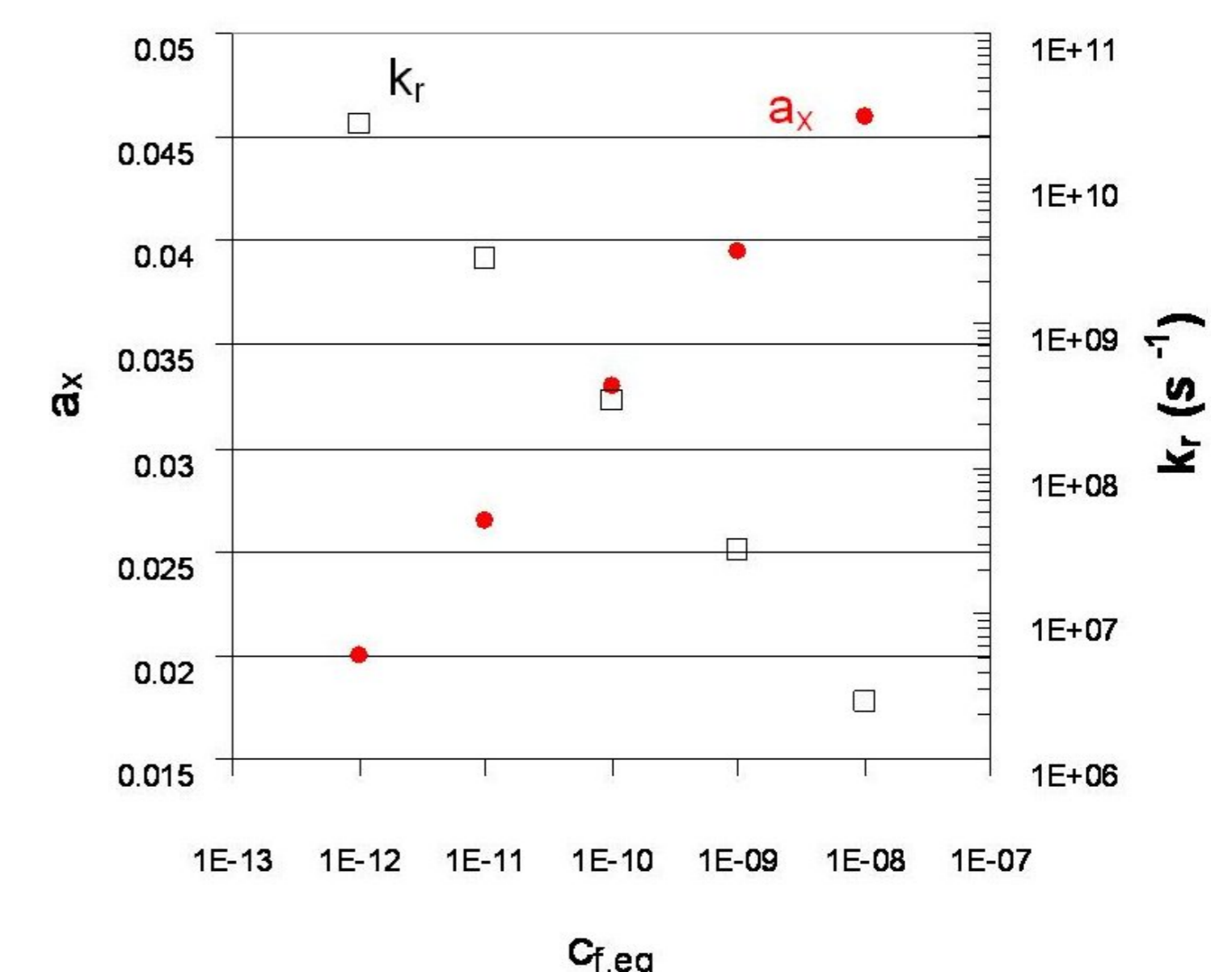


Figure 6: Dependency of a_x and k_r with $c_{f,eq}$ to get the same $\sigma(\epsilon)$ curve.

4.3 Deformation relaxation test

Model predicts rather accurately the dependency of $\Delta\sigma$ with relaxation time:

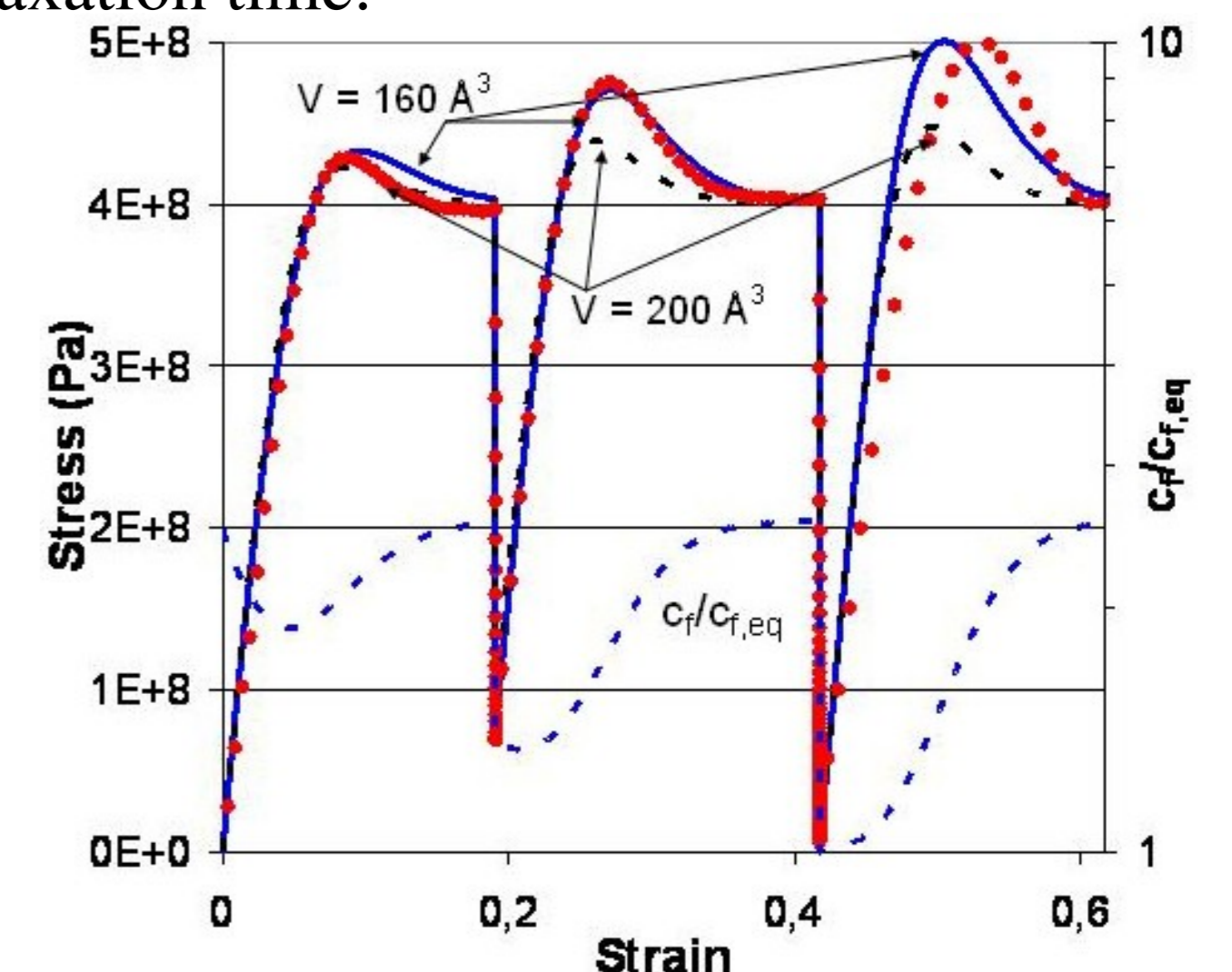


Figure 7: Comparison between model and experiment (deformation/relaxation test). $c_{f,i} = 2 \times c_{f,eq}$ and predicted variation of the relative flow defect concentration ($c_f/c_{f,eq}$)

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