The ultrasonic Bordoni peak in copper crystals and the kink picture

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Abstract. The ultrasonic logarithmic decrement and modulus defect in high purity copper crystals was measured at 10, 30 and 50 MHz in the temperature interval 5–373 K. The samples were deformed at room temperature in the 3–20% range along the ⟨111⟩ crystallographic direction. The experimental data were fitted over the whole interval of temperatures, assuming the contribution of two kink mechanisms: (i) relaxation by kink pair formation with diffusion in the dislocation line and (ii) overdamped resonance of the kink chain with a temperature dependent number of kinks in the dislocation lines. With this procedure both primary and secondary properties of the high frequency Bordoni peak could be satisfactorily explained. Numerical data are reported for peak parameters and for the kink diffusion coefficient.

1. Introduction

In 1949 Bordoni [1], measuring the internal friction of some FCC cold-worked metals at frequencies of ∼1 MHz, observed a relaxation peak at low temperatures. This peak is known as the Bordoni peak (BP), and was immediately related to the dislocations present in the metal. Later this peak was studied experimentally almost exclusively through internal friction measurements on a wide range of samples with different prior plastic deformation, cold work or crystal source [2]. But only a few works were devoted to the high MHz BP in copper. The most relevant ones are that by Niblett and Zein [3] for attenuation measurements at frequencies ⩽30 MHz and the present authors [4] for frequencies up to 50 MHz and in the interval of temperatures from 77 to 300 K.

In addition to the Bordoni peak there is a subsidiary peak at lower temperatures, first reported for copper by Niblett and Wilks and often referred to as the Niblett–Wilks peak. This peak is accepted as an inherent part of the relaxation phenomenon, closely related to the Bordoni peak [5]. It is usually designed as the Bordoni peak 1 (BP1) and the principal Bordoni peak as the Bordoni peak 2 (BP2). Although many efforts have been devoted to the motion of dislocations in crystals, the dynamics of dislocation lines driven by an oscillatory stress is not yet well understood [6]. In 1939 Peierls [7] made the first detailed calculus of the shear stress necessary to move a linear dislocation through the crystal lattice without thermal fluctuations (Peierls stress: σ_P). In 1952 Shockley [8] proposed that the existence of the Peierls potential should lead to the creation of kinks (i.e. short segments of the dislocation line in which the dislocation goes from one Peierls valley to another one)

and that they could be formed in thermal equilibrium. Later Seeger [9] considered that the thermally activated formation of kink pairs of opposite sign in an external oscillatory stress (KPF) would lead to an internal friction relaxation process. He also proposed that the relaxation peak observed by Bordoni in 1949 [1] in some plastically deformed FCC metals (known as the Bordoni peak (BP)) must be a consequence of this process. This model was successful on the prediction of the peak occurrence but fails for the secondary properties of the peak.

Seeger pointed out that also the Niblett–Wilks peak is due to KPF. The two types of dislocation that may lie along a ⟨110⟩ close packed direction originate both of the peaks in the FCC lattice. These are: one for which the Burgers vector is parallel to the dislocation line (a pure screw type) and the other for which the Burgers vector lies at $\pm 60°$ to the direction of the dislocation line. These two types of dislocation should have different values for the formation energy, and therefore for the activation energy for relaxation.

In 1981 Seeger [10] refined this first model including a kink diffusion mechanism in the KPF. The main characteristic of this model is the prediction of the existence of an effective activation enthalpy different for low and high temperatures and a temperature dependent relaxation time in both pre-exponential and exponential terms. Although this model predicts peaks broader than that obtained with the first model it is not complete enough to describe all experimental data [5, 10]. Bujard *et al* [11] showed in 1987 that the signature of kinks obtained from the KPF model closely corresponded to the internal friction obtained with the two-wave coupled technique in Al. This fact was interpreted as evidence that the Bordoni relaxation is originated by the KPF.

In addition to those kinks created by thermal activation, geometrical kinks [5] should be considered in dislocation lines not entirely lying in a Peierls valley. In dislocation lines almost parallel to crystallographic low index directions, fixed at pinning points situated in different Peierls valleys, these kinks are present even at very low temperatures. In 1964 Suzuki and Elbaum [12] considered that the kink chain could oscillate driven by an external oscillatory stress, presenting a resonant behaviour. In 1965 Alefeld *et al* [13] refined the model and proof that thermal kinks also should be included in the kink chain. These kinks should be produced at high temperatures also for zero applied stress.

As we showed in 1994 [14] the ultrasonic logarithmic decrement and its associated modulus defect should be considered as the superposition of this overdamped resonance and the relaxation (by KPF) component.

In 1995 Marchesoni [15] presented an attractive calculation of the logarithmic decrement in terms of kink mechanisms, in which the BP1, the BP2 and the background component are produced by the nucleation of kink pairs and kink migration. The principal BP was attributed to kink nucleation in the presence of a low density of geometrical kinks, in a similar way as in Seeger's model. The BP1 must be due to kink nucleation controlled by geometrical kinks, with an activation energy approximately half of that corresponding to the BP2. However, this model does not show the existence of the temperature dependence of the 'effective' activation enthalpy predicted by Seeger. For reasonable distributions in dislocation lengths also the predicted peaks remain thinner than those observed [15].

Finally, in 1996 Ulfert and Seeger [16] refined the KPF model taking into account the influence of geometrical kinks in KPF with kink diffusion. Although they found that the low frequency relaxation time was strongly dependent on internal stresses, the high frequency relaxation remains with the same temperature dependence as the previous model (i.e. with only thermal kinks in dislocation lines).

This paper is devoted to the measurement and result interpretation in terms of kink relaxation (KPF with kink diffusion) and resonance mechanisms, of the 10 to 50 MHz

logarithmic decrement δ and its associated modulus defect $\Delta M/M_0$ in high purity crystalline copper deformed in the range of 3–20%.

2. Experimental procedure

Four samples were prepared in a cubic form of approximately 1 cm side. All of them were cut from the same batch of crystals of high purity copper (RRR $\cong$ 1500). They were oriented in the $\langle 111 \rangle$ crystallographic direction better than $1°$, controlled by the Laue method.

The two faces used for ultrasonic measurements, with parallelism 10^{-4} rad, were polished with SiC and left in vacuum at $650°$C for 5 hours. The deformation at room temperature in the $\langle 111 \rangle$ direction was performed by compression in one step and then left for 1 hour at $100°$C. Each sample was prepared with a definite plastic deformation: 3, 5, 10 and 20%.

Ultrasonic attenuation and velocity were simultaneously measured using the conventional pulse-echo method [17]. This method was chosen because it enables the measurement of the attenuation and the velocity of pulses in the same sample for several frequencies. The elapsed time for a pulse round trip was accurately determined through the pulse-echo-overlap technique [18]. Nonaq stopcock grease was used as bonding between the quartz transducer (10 MHz fundamental frequency and 6.25 mm diameter) and the samples. All measurements were performed by cooling the sample from 373 K to 5 K, at a maximum rate of 1 K min^{-1}. After each cooling the sample was left at $100°$C for 1 hour.

The logarithmic decrement δ and the modulus defect $\Delta M/M_0$ were calculated with the following equations:

$$\delta = 0.115 \frac{\alpha - \alpha_0}{f \, (\text{MHz})} \tag{1}$$

$$\frac{\Delta M}{M_0} = \frac{v^2 - v_0^2}{v_0^2} \tag{2}$$

where $f \, (\text{MHz})$ = wave frequency expressed in megahertz; α_0 = attenuation and v_0 = velocity of ultrasonic pulses measured in a dislocation-free sample (background); α = attenuation and v = velocity of ultrasonic pulses measured in the non-irradiated samples. Eiras [19] measured α_0 and v_0 in a $\langle 111 \rangle$ non-deformed copper sample, irradiated with γ-rays until total pinning of dislocations. We assume this background, including its temperature dependence, valid for our deformed samples.

3. Experimental data

In figure 1 we present the attenuation versus temperature measured in our samples, at frequencies of 10, 30 and 50 MHz. This figure show the presence of the two peaks known in the literature [5, 6] as the BP1 (or Niblett and Wilks peak) and BP2 (or Bordoni peak). The BP1 is observed at lower temperatures than the BP2, and it is always smaller than the BP2. Outside the peak, the 'hot' side of the BP2 shows an increase of the attenuation with temperature. At temperatures below 50 K an increment in attenuation was observed, which is stronger for higher frequencies. It is attributed in the literature [5] to the interaction of dislocation lines with the free electrons in the crystal.

In figure 2 we present representative curves of the modulus defect and its associated logarithmic decrement plotted versus temperature. All the modulus defect curves show the characteristic step of a relaxation process [5], the largest for the 20% deformed sample.
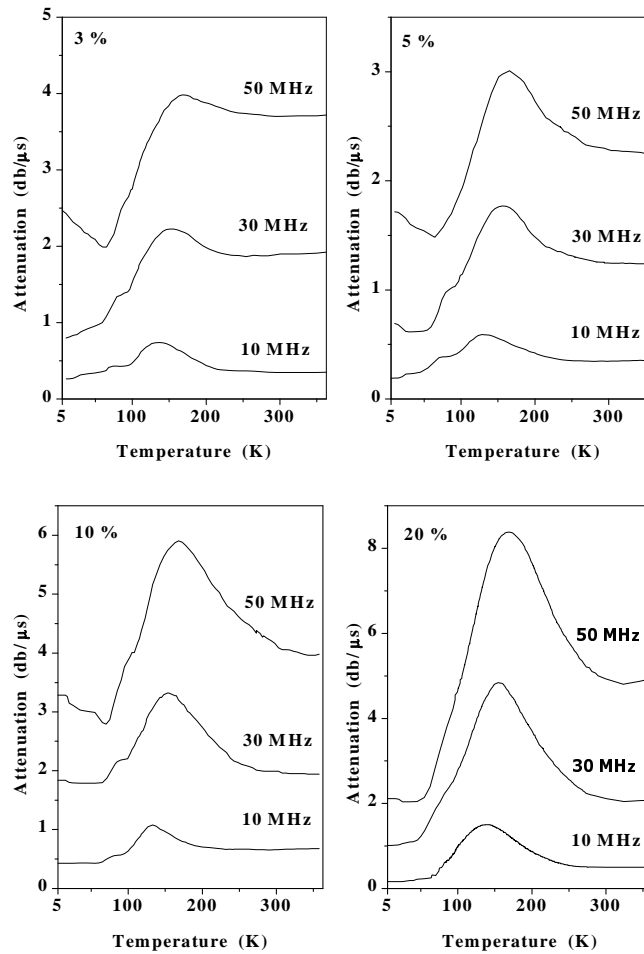
Figure 1. Ultrasonic attenuation as a function of temperature, measured at 10, 30 and 50 MHz in samples deformed by compression in $\langle 111 \rangle$ between 3 and 20%. The sample was cooled at a rate of 1 K min^{-1}.

4. Theoretical considerations

As we show in this paper, the logarithmic decrement and the modulus defect are well fitted if they are considered to be due to the simultaneous contribution of both relaxation and resonance of dislocations in the crystal. The dislocation relaxation is considered to be composed of two individual relaxation components for the BP1 and the BP2, the resonance being a single process for the whole interval of temperatures studied in this report. The two relaxation peaks, as Seeger earlier pointed out, originate in the FCC lattice from the two types of dislocation which may lie along a $\langle 110 \rangle$ close packed direction. There is one for which the Burgers vector is parallel to the dislocation line (a pure screw type) and the other for which the Burgers vector lies at $\pm 60°$ to the direction of the dislocation line. These two types of dislocation should have different values for the formation energy and therefore for the activation energy for relaxation.

Each relaxation component is considered to be originated by kink pair formation (KPF). Assisted by the external stress the kink pairs are formed in thermal equilibrium by thermal
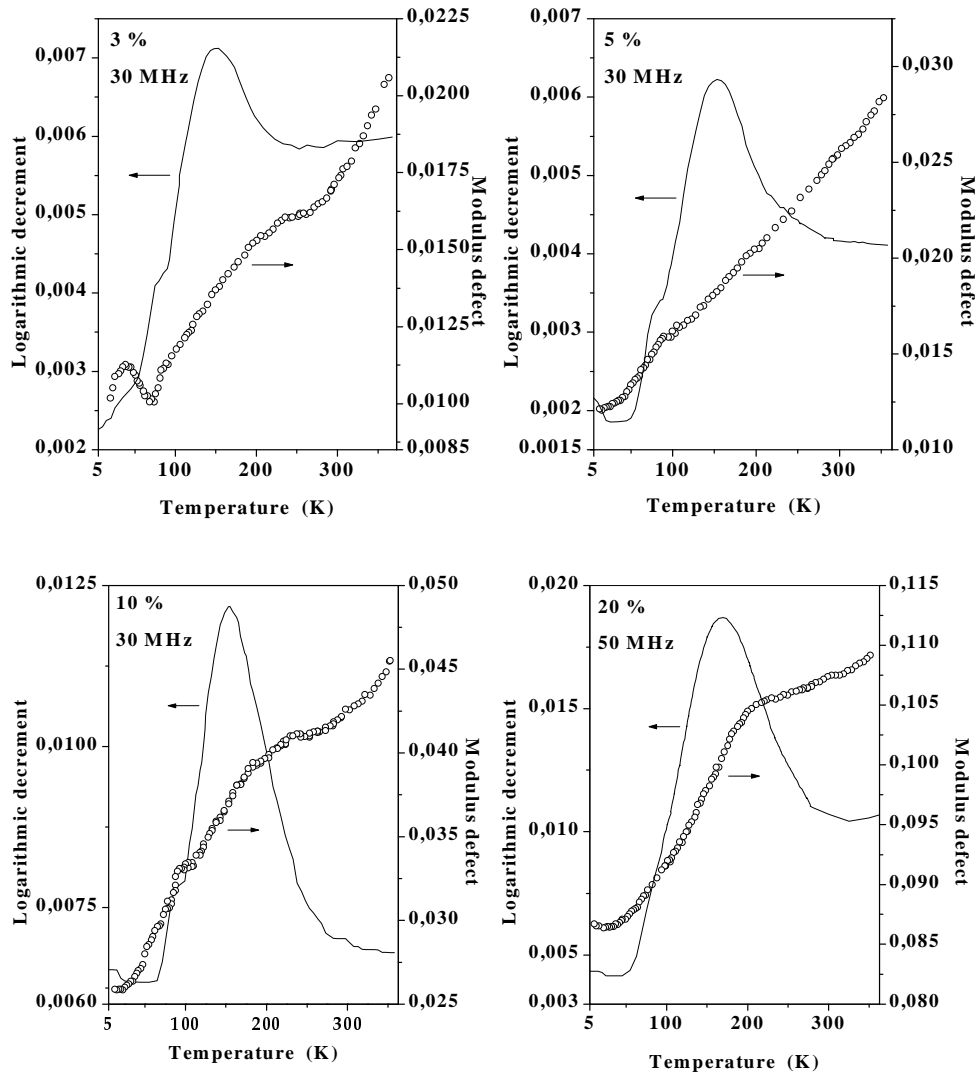
Figure 2. Some representative logarithmic decrements and associated modulus defects as a function of the temperature, for the samples of figure 1.

activation. In agreement with Seeger [10] the relaxation time associated with this process is given by

$$\tau = \frac{k_B L}{\pi w_k H_k} \frac{T}{D_k} \frac{(1 + \rho_k^{eq} L/2)}{(\rho_k^{eq})^2} \tag{3}$$

where L = average free length of segment of the dislocation line; w_k = kink width; H_k = half the activation enthalpy of the formation of kink pairs; D_k = kink diffusion coefficient and ρ_k^{eq} = average density of kinks in thermal equilibrium on the dislocation. For temperatures above $\theta_D 2a/\pi w_k = 44$ K ($\theta_D = 343$ K = Debye temperature of copper; a = interatomic distance in the dislocation line direction and $w_k = 20a$), the high temperature approximation

for ρ_k^{eq} is applied,

$$\rho_k^{eq,ht} = \frac{1}{w_k}\left(\frac{2\pi H_k}{2k_B T}\right)\exp\left(\frac{-H_k}{k_B T}\right). \tag{4}$$

In agreement with equation (3) the activation enthalpy appears depending on temperature and should be calculated as an effective enthalpy,

$$H_{ef} = \frac{d(\ln \tau)}{d(1/k_B T)}. \tag{5}$$

Equation (5) has two important approximations: low temperatures ($\rho_k^{eq}L \ll 1$) for which $H_{ef} = 2H_k - 2k_B T \cong 2H_k$, and high temperatures ($\rho_k^{eq}L \gg 1$) for which $H_{ef} = H_k - \frac{3}{2}k_B T \cong H_k$. These approximations point out an important feature predicted by the model: the effective activation energy is very different for the low and high frequency BP. As proposed by Seeger [10], the effective high temperature activation energy closely corresponds to the energy necessary to create an isolated kink W_k, and the low temperature one to the energy necessary to create a kink pair, $2W_k$.

A second important feature is due to the temperature dependence of the pre-exponential relaxation time coefficient: the obtained relaxation peak should be broader than a single Debye peak [10]. This fact becomes very important considering that experimental BPs are broader than a Debye peak, as we showed earlier [14].

The temperature behaviour of the modulus defect outside the peak region strongly suggested the existence of a resonant component superposed on the relaxation. In terms of kinks, this resonant mechanism should be attributed to the kink chain (formed by geometric and thermal kinks) oscillations.

As proposed by Alefeld *et al* [13], thermal kinks will be produced without an applied stress at temperatures above the critical temperature T_c

$$T_c = \left(\frac{H_k}{k_B}\right)\ln\left[\frac{2a(1+N_0)^{1/2}}{AL}\right]. \tag{6}$$

We assume that these kinks should contribute to the kink chain resonance, given a temperature dependence of kink density for temperatures above T_c. This temperature, calculated by Alefeld [13], is around 115 K for copper if $N_0 \approx 15$ is assumed.

Due to the simultaneous contributions of both relaxation 1 and 2 and the resonance, the general expression for the modulus defect and logarithmic decrement becomes,

$$\frac{\Delta M}{M_0}(T) = \left(\frac{\Delta M}{M_0}\right)_{B1} + \left(\frac{\Delta M}{M_0}\right)_{B2} + \left(\frac{\Delta M}{M_0}\right)_{RESONANCE}$$

$$= \Delta_{B1}\frac{1}{1+(\omega\tau_1)^2} + \Delta_{B2}\frac{1}{1+(\omega\tau_2)^2} + A_1 N(T)L^2 + \frac{\Delta M}{M_0}$$

$$= \Delta_{B1}\frac{1}{1+(\omega\tau_1)^2} + \Delta_{B2}\frac{1}{1+(\omega\tau_2)^2} + B_1 T + \frac{\Delta M}{M_0} \tag{7}$$

$$\delta(T) = \delta(T)_{B1} + \delta(T)_{B2} + \delta(T)_{RESONANCE}$$

$$\pi\Delta_{B1}\frac{\omega\tau_1}{1+(\omega\tau_1)} + \pi\Delta_{B2}\frac{\omega\tau_2}{1+(\omega\tau_2)} + A_2 N(T)L^4\omega B(T) + \delta_0$$

$$= \pi\Delta_{B1}\frac{\omega\tau_1}{1+(\omega\tau_1)} + \pi\Delta_{B2}\frac{\omega\tau_2}{1+(\omega\tau_2)} + B_2 T^2 + \delta_0 \tag{8}$$

$$\tau_{1/2} = B_{3(1/2)}(k_B T)^{3/2}\exp\left(\frac{H_{k(1/2)}}{k_B T}\right) \tag{9}$$

where $\Delta_{B1/2}$ are the Bordoni relaxation intensity of the BP1 and BP2 relaxation respectively, ω is the wave angular frequency and A_1, A_2, B_1, B_2 and $B_{3(1/2)}$ are constants which depend on the
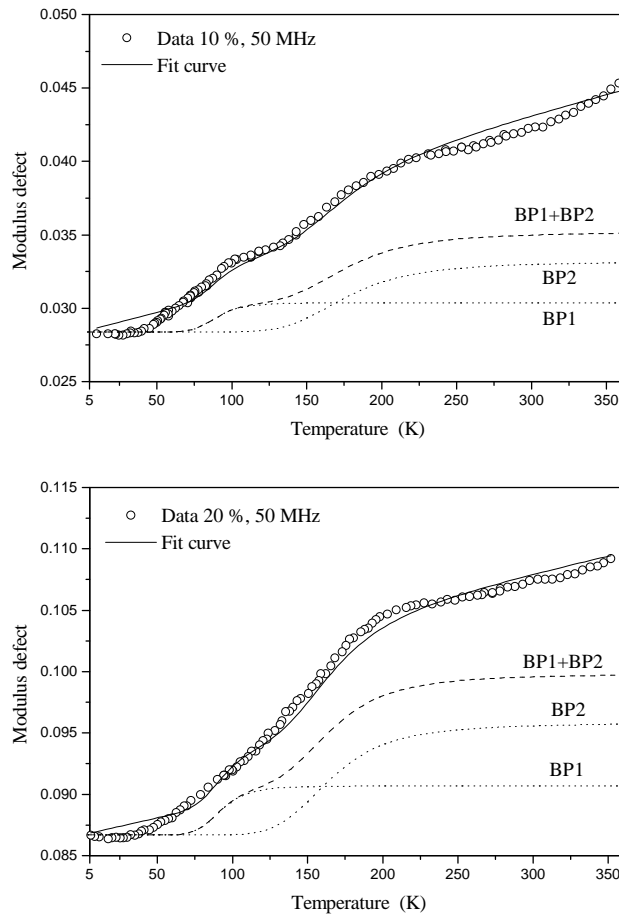
Figure 3. Some representative fits of modulus defect with the equations (7) and (9). The BP1 and BP2 relaxation are shown separately. The sum of BP1 and BP2 is also shown.

material and the dislocation structure. Different activation enthalpies $H_{k(1/2)}$ are considered for the relaxation 1 and 2, respectively.

As we previously showed [14] the behaviour of the logarithmic decrement and modulus defect near room temperature strongly suggest that a low frequency approximation for the overdamped resonance should be considered. In this approximation they become [12]

$$\delta \propto N(T)L^4\omega B(T) \tag{10}$$

$$\Delta M/M_0(T) \propto N(T)L^2. \tag{11}$$

The modulus defect in equation (11) is only dependent on temperature through $N(T)$. As the experimental modulus defect increases approximately linearly above BP2 temperatures, we assumed for $N(T)$ a direct proportionality with T. This relation is used in this report for fitting purposes in all the temperature range investigated. For the overdamped coefficient for copper Eiras [19] found experimentally $B(T) \propto T$.

As is well known [5], in the overdamped resonance of the kink chain the mass term becomes unimportant and the dynamical behaviour becomes that for a standard anelastic solid as reflected in our equations for the resonance.
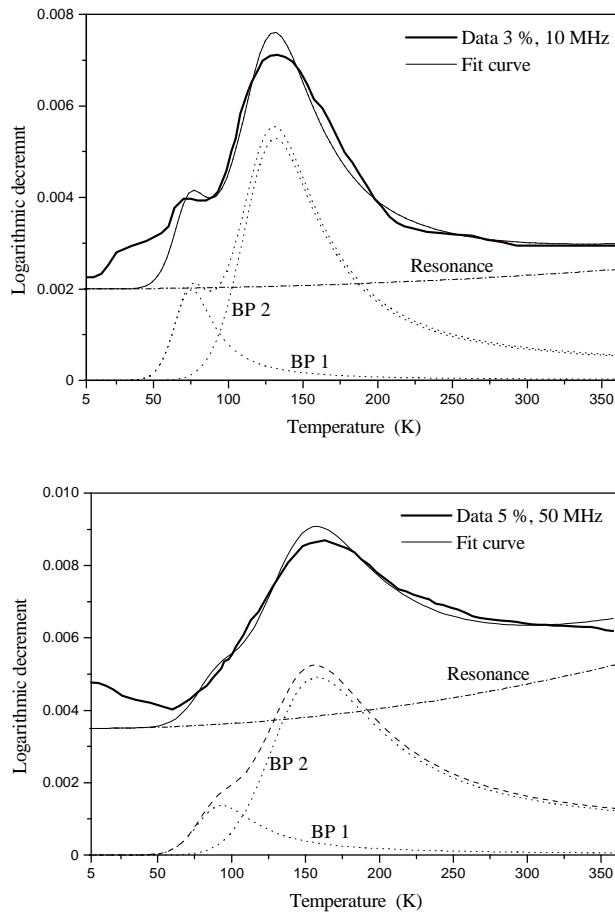
Figure 4. Some representative fits of logarithmic decrement with equations (8) and (9), for the samples of figure 1. The relaxations BP1 and BP2 and the resonance component are shown separately. The traced curve represents the sum of BP1 and BP2.

5. Fits and discussion

Figures 3 and 4 show typical curves of the modulus defect and logarithmic decrement versus temperature, respectively, fitted with equations (7) to (9). All fits in this paper were realized using a standard fitting program.

Figure 3 points to the importance of the resonant mechanism responsible for the variation of the modulus defect outside the step region of kink relaxation and the assumption $N(T) \propto T$ is justified in the temperature range investigated in this paper. From these fits primary values for the relaxation intensity were obtained, which were then used in the fits performed over logarithmic decrement allowing only minor variations in this parameter.

All fitted curves in figure 4 look very close to the experimental data. As we showed [14], if a simple Debye relaxation time is considered for Bordoni relaxation taking a similar addition of mechanisms, the experimental peaks are always broader than the fitted peaks. This problem is now resolved, the relaxation time becoming very important in equation (9).
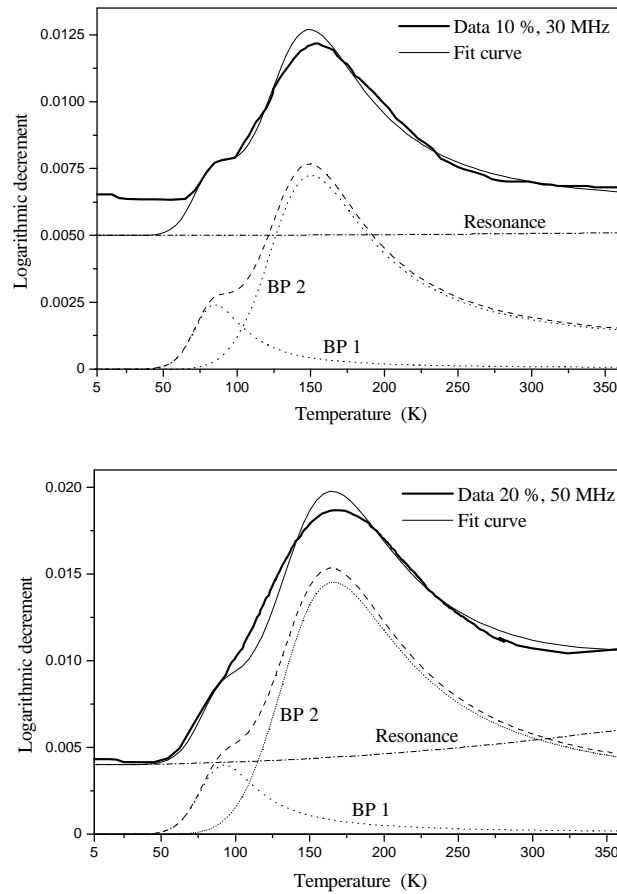
Figure 4. (Continued)

In figure 5 we show an Arrhenius plot with peak temperatures assembled for copper from [1, 20–31] and those obtained by us for high temperatures and for low temperatures in samples cut from the same crystal batch [4, 32]. The peak temperatures in this plot run from 50 K to 170 K covering the lowest and the highest peak temperatures achieved from Bordoni peaks. This plot is well fitted with the relaxation time for the KPF mechanism (equations (3) and (4)). In this fit H_k and D_k were left to freely vary with the other parameters closely kept on values $L \sim 10^4 a$, $w_k \sim 20a$ and $a \sim 3.5 \times 10^{-8}$ cm [33]. The estimated parameters from this fit are: $H_k = (0.075 \pm 0.001)$ eV and $D_k = (2.91 \pm 0.07)$ cm^2 s^{-1}.

The most important feature of this fit is the existence of an 'effective' activation enthalpy, which varies from 0.075 eV for the highest temperatures to 0.15 eV for the lowest temperatures. In the literature for the BP in copper the commonly accepted value for $2H_k$ is 0.12 eV [5, 6], which is 25% lower than obtained in this paper.

The existence of this 'effective' activation energy lets us disregard the model proposed by Marchesoni [15] because it does not predict this well confirmed behaviour.

The Peierls stress σ_P can be evaluated from the line tension model and experimental data for the activation energy [6]. With $2H_k = 0.1$ eV for copper, Benoit *et al* [34] obtained $\sigma_P = 20$ MPa. With the activation energy of 0.15 eV obtained by us the same calculus leads
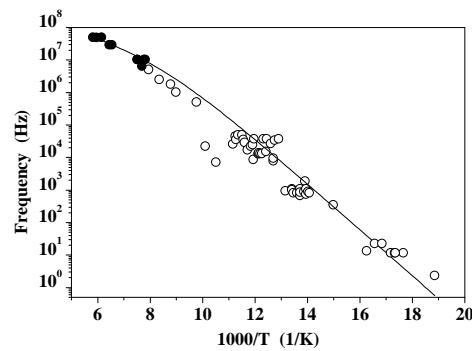
Figure 5. Arrhenius plot for copper and its fitted curve (equations (3) and (4)). The peak temperatures are from this paper (solid circles) and [1], [20]–[33] (open circles).
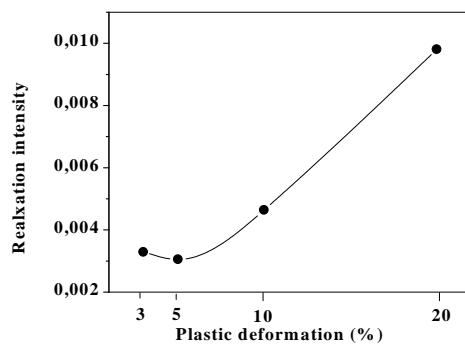

Figure 6. Relaxation intensity for copper as a function of the plastic deformation. The relaxation intensity was obtained from the BP2 fitted relaxation component (equations (8)).

to $\sigma_P = 30$ MPa. These values are too high if compared with the critical resolved shear stress (σ_0) for copper measured near liquid helium temperature ~ 1 MPa [6]. This discrepancy leads to some doubts about the interpretation of the BP in terms of KPF, because at low temperatures the formation of thermal kinks becomes negligible and then the critical resolved shear stress should equal the Peierls stress. Benoit *et al* [34] explained this difference, proposing the existence of a short-circuit mechanism for dislocation lines, originating in kinks formed in partial dislocations in the presence of point defects. Later Gremaud *et al* [35] refined this mechanism. In order to obtain an independent value of the Peierls stress, we also calculated σ_P by computational techniques, finding a value close to 30 MPa for copper [36]. Nevertheless this point remains as one for further discussion and some authors, such as Schoeck [37] and Okuda [38], pointed out the importance of partial dislocations present in FCC crystals in explaining the difference between σ_P and σ_0.

In figure 6 we present a plot of the relaxation intensity versus sample deformation. The relaxation intensity was obtained from the component BP2 in each fitted curve on logarithmic decrement, which are accurate values also for those curves presenting high asymmetry. This figure shows the relaxation intensity decreasing between 3 and 5% and then increasing monotonically with the sample deformation in the interval from 5 to 20%. The minimum in the relaxation intensity at 5% corresponds to the minimum previously observed in the peak temperature at this deformation [19].

The peak width is calculated from the logarithmic decrement relaxation component as $(E/k_B)(1/T_1 - 1/T_2)$. E is the activation energy of the process, obtained as the 'effective' energy from the Arrhenius plot, and T_1 and T_2 are the temperatures at which the logarithmic decrement falls to 0.5 times the peak value. A width of 1.3 times the Debye peak for every BP2, independent of sample deformation and frequency, is obtained.

6. Conclusions

- A good agreement between ultrasonic logarithmic decrement and modulus defect experimental data and the model proposed in this paper is obtained, corresponding to the simultaneous contribution of KPF with kink diffusion and the overdamped resonance of the kink chain. It takes into account the primary and the secondary properties of the ultrasonic BP.
- Half the activation enthalpy of the formation of kink pairs $H_k = (0.075 \pm 0.001)$ eV. The temperature-dependent 'effective' activation enthalpy ranges from 0.075 eV at high frequencies to 0.15 eV at low frequencies.
- The peak width, 1.3 times the Debye peak, is independently obtained from sample deformation and frequency.
- The relaxation intensity shows a slight minimum at approximately 5% and a monotonic increase with sample deformation in the investigated range (<20%).
- The kink diffusion coefficient for copper crystals is $D_k = (2.91 \pm 0.07)$ cm^2 s^{-1}.

Acknowledgments

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