Internal Friction by Pinned Dislocations: Theory of the Bordoni Peak

F. Marchesoni*,†
Department of Physics, Boston University, Boston, Massachusetts 02215
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The two most prominent internal friction peaks in cold worked metals at low temperature are shown to be related manifestations of the same nucleation mechanism of kink-antikink pairs in pinned dislocation segments depending, respectively, on the absence (Bordoni peak) or the presence (Niblett-Wilks peak) of geometrical kinks (antikinks). Correspondingly, diffusion of the nucleated thermal pairs accounts for the observed background internal friction. Peak and background components are both computed analytically and compared with experimental data.

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Almost fifty years ago Bordoni [1] found that fcc metals (single crystals or polycrystalline specimens alike) subjected to cold work develop a prominent maximum in the curve of internal friction versus temperature in the range 50–100 K. Ensuing investigations led to a detailed experimental characterization of the phenomenon, which can be summarized as follows [2,3]. (a) The Bordoni peak is absent in well annealed samples; its height increases with the amount of cold work for deformations up to 3% and remains fairly constant for larger deformations. (b) Annealing after cold work reduces the height of the peak (more markedly on the high-temperature side) but does not eliminate it until recrystallization occurs. (c) The temperature T_B of the peak maximum increases almost logarithmically with the vibration frequency, as expected if the peak were the signature of a thermally activated relaxation process. (d) The height of the peak is reduced by the presence of impurities and by massive neutron irradiation; T_B is not affected significantly in either case.

The shape of the Bordoni peak has been baffling both experimentalists and theoreticians since. Its width is several times larger than that corresponding to a single relaxation process. In addition, there is a subsidiary peak (sometimes just a shoulder) at lower temperatures often referred to as the Niblett-Wilks (NW) peak [2]. The observation that the NW peak decreases almost proportionally with the Bordoni peak, e.g., during annealing, indicates a close relationship between the two peaks.

Items (a)–(d) are all suggestive of a dislocation mechanism [4] at work. A dislocation segment which lies along a Peierls valley can overcome the relevant confining barriers (quantified by the Peierls stress σ_P) only by nucleating a kink-antikink pair. Nucleation is a thermally activated phenomenon and contributes to the internal friction with a Debye peak, the frequency constant which coincides with the nucleation rate in the dislocation segment. Such a model was introduced first by Seeger and Schiller [5]. Refinements [4–8] of the original theory did not help dispell a few serious criticisms to the model, namely [3,4], (i) the theory predicts a dependence of T_B on the vibration amplitude, which was never observed experimentally; (ii) the width of both the Bordoni and the NW peak could not be reproduced by a single nucleation process; (iii) a substantial fraction of the dislocation network is known to contribute to the Bordoni relaxation [3,7], at variance with the idea that only dislocations parallel to the Peierls valleys are involved; (iv) no relation between main and subsidiary peaks it envisaged; and (v) the theory omits an explanation of the rise in the background internal friction which follows both peaks [7].

In the present Letter we develop an analytical treatment of thermal relaxation in a pinned dislocation segment. Application to the internal friction problem leads us to a natural interpretation of the Bordoni peak, thus accounting for all items (i)–(v) without unnecessary assumptions.

We agree to represent the position of a dislocation line in its glide plane as a sine-Gordon (SG) string $\phi(x,t)$ coupled to an equilibrium heat bath, that is [4,5],

$$\phi_{tt} - c_0^2\phi_{xx} + \omega_0^2 \sin\phi = -\alpha\phi_t + \zeta(x,t), \quad (1)$$

where c_0 and $\omega_0 \equiv 2\pi\nu_0$ are the parameters of the unperturbed SG equation, the sinusoidal potential $-\omega_0^2\cos\phi$ models a system of parallel Peierls valleys, α denotes the damping constant, and the Gaussian noise $\zeta(x,t)$ has zero mean and correlation function

$$\langle\zeta(x,t)\zeta(x',t')\rangle = 2\alpha kT\delta(x-x')\delta(t-t'). \quad (2)$$

If a dislocation line is pinned between two points, e.g., at $x = 0$ and $x = l$, each lying at the bottom of two Peierls valleys, then $\phi(l,t) - \phi(0,t) = \pm 2\pi|m|$, with $m = 0, \pm 1, \pm 2\ldots$, and the corresponding dislocation segment of length l is said to bear m geometrical kinks ϕ_+ or antikinks ϕ_-, depending on the signs $\pm$, respectively. Throughout this Letter we assume that the half-width of $\phi_\pm$, $d = c_0/\omega_0$, is small compared with the average separation between their centers (*dilute gas approximation*) [9]. It is well known that, due to the perturbation on the right-hand side of Eq. (1), a single kink (antikink) behaves like a quasiparticle of rest energy $E_0 = 8\omega_0 c_0$ (i.e., mass E_0/c_0^2) subject to a Brownian motion with diffusion constant $D = (kT/E_0\alpha)c_0^2$ [9,10]. Let us restrict ourselves to the *underdamped limit* $\alpha \ll \omega_0$, [11] as indicated by both theory [12] and direct

measurements [13] of the dislocation viscous forces. In such a limit a kink and an antikink approaching from infinity will eventually pass through each other with a small fractional energy loss $\delta(\alpha) \simeq \pi^2\alpha/\omega_0$, whereas two kinks (antikinks) bounce off one another almost without dissipation [11].

Before proceeding any further we remind the reader that, to make contact with a real dislocation, lattice units must be restored in Eq. (1), i.e.,

$$\phi \to a\phi/2\pi\,, \quad c_0^2 \to C/\pi p a^2\,, \qquad \omega_0^2 \to 2\sigma_P b/\rho a^3\,, \quad \alpha \to B/\pi\rho a^2\,, \tag{3}$$

where a is the lattice constant, b is the Burgers vector, ρ is the density of the material, B and $C \simeq Gb^2$ are the viscous and the tension forces per unit of dislocation length, respectively, and G is the shear modulus. In passing, we also note that the coupling of the lattice phonons with the highly nonlinear core of the dislocation line is responsible for the temperature dependence of B [12], i.e.,

$$\alpha(T) = \alpha(0) + \gamma(kT/E_0)\,. \tag{4}$$

In the temperature range of interest, here $\alpha(0)$ can be neglected and γ determined experimentally [13].

Internal friction in a sample subjected to a small periodic external stress with frequency $\nu = \omega/2\pi$ is defined by the ratio $\Delta(\omega, T)$ of the energy lost per radian to the maximum stored energy [3,4]. The microscopic dissipation mechanism is due to the damped dislocation segments bowing out in the direction of the on-plane perpendicular component $\sigma(t)$ of the applied bias. At high temperatures $kT \gg E_0$, we can approximate $\sigma_P = 0$, thus recovering the vibrating string model by Granato and Lücke [14]. The Bordoni peak, instead, occurs for $kT \ll E_0$, so that the Peierls potential plays a crucial role. Indeed, a SG string under the action of the bias $F = -ab\sigma(t)/2\pi$ bows out according to two distinct mechanisms, pair nucleation and kink (antikink) diffusion, as explained below.

Pair nucleation.—Thermal noise generates kink-antikink pairs even in the absence of an external bias [9–11], as proven by the fact that at low temperatures the density of thermal kinks (antikinks) [15]

$$n(T) = \left(\frac{2}{\pi}\right)^{1/2} \frac{1}{d}\left(\frac{E_0}{kT}\right)^{1/2} \exp\left(-\frac{E_0}{kT}\right) \tag{5}$$

is independent of both F and m. On the other hand, the bias F pulls $\phi_\pm$ apart by exerting opposite forces $\pm 2\pi F/c_0^2$ on them [9]. As a consequence, the nucleation of an additional pair at thermal equilibrium makes the SG string shift an average distance π in the direction of $\sigma(t)$. [We recall that in the units of Eq. (1) 2π denotes the intervalley spacing.]

Kink (antikink) diffusion.—Diffusion of a single underdamped kink (antikink) from one pinning point to the other causes the SG string to advance by a quantity 2π. Because of the collisional properties mentioned above, this holds even in the presence of a gas of kinks and antikinks, each gas component being related here as if it were made of indistinguishable quasiparticles [10,11]. Of course, F selects shifts in the direction of $\sigma(t)$. Actually, the diffusion process involves geometrical and thermal kinks (antikinks) alike. However, the former ones, in view of their reduced mobility as a whole, simply generate the internal friction component already predicted by the vibrating string model [16]. At low frequencies such a component is small [17] and exhibits a weak T dependence [14], so that it can be easily subtracted [7]. The contribution of thermal pairs, instead, depends on T through the density function $n(T)$ and is not quenched by geometrical constraints.

We now calculate the frequency constants for both relaxation processes in a pinned dislocation segment of length l bearing m geometrical kinks (antikinks) by generalizing the approach of Ref. [11]. Let $n_\pm(T)$ denote the *total* density of $\phi_\pm$ in the SG string. An underdamped kink (antikink) $\phi_\pm$ diffuses a root mean square distance $[n_\pm^2\delta(\alpha)]^{-1/2}$ before annihilating in a time interval $\tau_\pm$. In the same time interval an underdamped Brownian particle would diffuse a root mean square distance $(\alpha D)^{1/2}\tau_\pm$, where the kink (antikink) lifetime $\tau_\pm = [\alpha\delta(\alpha)n_\pm^2]^{-1/2}$. The pair nucleation rate over the entire string length is then readily written as

$$\Gamma_n = l(n_+/\tau_+ + n_-/\tau_-) = 2l[\alpha D\delta(\alpha)]^{1/2} n_+ n_-\,. \tag{6}$$

Accordingly, the time τ_0 taken by a kink or an antikink to diffuse a rms distance equal to the string length l in the underdamped limit is $\tau_0 = l/(\alpha D)^{1/2}$ where the total diffusion rate of kinks and antikinks towards the string pinning points is

$$\Gamma_d = l(n_+ + n_-)/\tau_0 = (\alpha D)^{1/2}(n_+ + n_-)\,. \tag{7}$$

It will be shown later that the nucleation and diffusion of thermal kinks (antikinks) is responsible for the peak and the background component of the internal friction, respectively. The relevant frequency constants can be derived from Eqs. (6) and (7) and rewritten as [see Eqs. (4) and (5)]

$$\nu_B(T) = \Gamma_n/2\pi = \nu_B^0[1 + m/\ln(T)]\exp(-2E_0/kT)\,, \tag{8}$$

with $\nu_B^0 = 4(l/d)(\gamma/\omega_0)^{1/2}\nu_0$ and

$$\nu_b(T) = \Gamma_d/2\pi = \nu_b^0[1 + m/2\ln(T)]\exp(-E_0/kT)\,, \tag{9}$$

with $\nu_b^0 = 2(2/\pi)^{1/2}\nu_0$. Note that at variance with Ref. [5], ν_B^0 and ν_b^0 do not depend on the amplitude of the periodic bias $\sigma(t)$ [see item (i) above]. Moreover, both ν_B^0 and ν_b^0 are independent of the temperature as suggested first by Bordoni and co-workers [1]. The temperature dependence of the attack frequencies in Eqs. (8)

and (9) is determined by the interaction of thermal and geometrical kinks and antikinks. The ratio ν_B^0/ν_b^0 can be easily expressed in terms of the lattice constants, i.e., $\nu_B^0/\nu_b^0 = (l/d)(\gamma/\nu_0)^{1/2}$.

The calculation of the internal friction in terms of the microscopic relaxation constants (8) and (9) is now straightforward. The formalism of Refs. [4,6,18] can be easily generalized to account for both relaxation mechanisms. That leads us to the following expression for the internal friction generated by a dislocation segment of length l bearing m geometrical kinks (antikinks):

$$\Delta_{lm}(\nu,T) = \Delta_0(T) l^3 \left[\frac{\nu \nu_B(T)}{\nu^2 + \nu_B^2(T)} + 2\frac{\nu \nu_b(T)}{\nu^2 + \nu_b^2(T)} \right], \quad (10)$$

with $\Delta_0(T) = a^2 b^2 G n(T)/4kT$.

Finally, we must add up the contributions from each segment in the dislocation network. This can be done by first averaging Δ_{lm} over m for a given value of l and, then, integrating the result thus obtained against an appropriate distribution $P(l)$ of the segment lengths. For simplicity, we assume here that all orientations of a segment of length l are equally probable, with the restriction that the segment cannot bear more than a maximum number M_l of kinks (antikinks), lest it becomes unstable towards unpinning [17]. Furthermore, we adopt the most popular expression for $P(l)$, that is $P(l) = (\Lambda/L^2)\exp(-l/L)$, where L is the average segment length and Λ is the dislocation density or dislocation line length per unit of volume. Recall that Λ depends strongly on the treatment, thermal and mechanical, undergone by the sample.

In Fig. 1 we plot separately the peak $\Delta_B(T)$ and the background component $\Delta_b(T)$ of the internal friction versus temperature for $\nu = 1.6 \times 10^4$ Hz and the lattice parameters of copper [19]. Far from trying the best fit of any particular set of experimental data, we limit ourselves to a few general (and concluding) remarks.

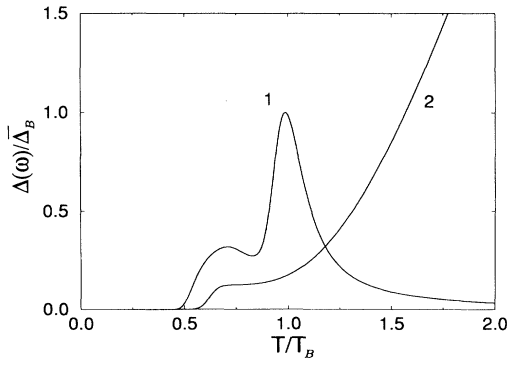

FIG. 1. Example of the peak (curve 1) and the background component (curve 2) of the internal friction for reasonable values of the lattice parameters (lightly cold worked copper [19]). The scales $\bar{\Delta}_B$ and T_B are discussed in the text.

$\Delta_B(T)$ exhibits a main peak for $T_B = 70$ K and a side peak of relative height 0.3 at $T_{NW} = 50$ K. The two peaks appear simultaneously upon averaging over m. The physical meaning of this result is clear: The main peak (the Bordoni peak) originates from pair nucleation in the presence of the low density of geometrical kinks (antikinks), such as in Seeger's theory; the subsidiary peak (to be interpreted here as the so-called Niblett-Wilks peak) is revealing of a geometrical kink (antikink) controlled nucleation process, whose effective activation energy, not surprisingly, is of the order of half the Bordoni energy [19].

The peak structure of Fig. 1 is about 20 K wide, fairly irrespective of the averaging constants M_l and L. This is quite an improvement with respect to earlier theories [2–4]. At present it is still unclear whether the width of $\Delta_B(T)$ can be further increased to match the experimental values (35 K or more) through more realistic averaging procedures, or we must advocate additional contributions from other types of lattice dislocations with slightly different activation energies [5,7]. This question is a matter of ongoing research.

The background contribution $\Delta_b(T)$ presents a striking resemblance to Thompson and Holmes' experimental data (see Fig. 15 of Ref. [7]). The residual internal friction rises sharply immediately after each peak of $\Delta_B(T)$ (see Ref. [7] for a physical interpretation of this phenomenon). Both jumps in $\Delta_b(T)$ occur on an energy scale of the order of the kink rest energy [4]. Note that no adjustable parameter in the present theory allows us to shift $\Delta_b(T)$ along the T axis relative to $\Delta_B(T)$.

The maximum number of geometrical kinks (antikinks) which can be accommodated in a dislocation segment of length l without generating internal stresses due to their mutual repulsion [6] is $\bar{M}_l = l/2d$. We verified that, when averaging Eq. (10) with respect to m, the amplitude of the Bordoni peak relative to the background is almost independent of M_l for $M_l > 0.4\bar{M}_l$. On decreasing M_l below that value the rising branch of $\Delta_b(T)$ fades away first, thus making the Bordoni peak shoot up from the background. For $M_l < 0.2\bar{M}_l$ $\Delta_B(T)$, too, becomes sensitive to the choice of M_l. This means that as much as 20%–40% of the dislocation network contributes to a certain extent to the Bordoni relaxation, in agreement with earlier experimental studies [3,7].

The ratio of $\Delta_B(T)$ to $\Delta_b(T)$ is approximately inversely proportional with L; see Eqs. (8)–(10). The values of M_l ($= 0.6\bar{M}_l$) and L ($= 10^{-4}$ cm) adopted in Fig. 1 are fairly adequate for the lightly cold worked samples tested in Ref. [7]. Larger amounts of cold work are expected to diminish both L (i.e., modify [18]) and $M_l/\bar{M}_l$, thus making the Bordoni peak grow more pronounced [15,20]. Finally, we remark that the Bordoni peak height $\bar{\Delta}_B \simeq 5 \times 10^{-3}$, reported in Ref. [7], can be reproduced in the present formalism by choosing a dislocation density Λ in the range of 10^8–10^9 cm^{-2}.

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*Mailing address: Istituto Nazionale di Fisica Nucleare, VIRGO Project, Università di Perugia, I-06100 Perugia, Italy. Electronic address: marchesoni@perugia.infn.it

†On leave of absence from Dipartimento di Matematica e Fisica, Università di Camerino, I-62032 Camerino, Italy.

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