Unlocking of an Elastic String from a Periodic Substrate

C. Cattuto
Dipartimento di Fisica, Universitá di Perugia, I-06100 Perugia, Italy

F. Marchesoni
Department of Physics, University of Illinois, 1110 West Green St, Urbana, Illinois 61801
and Istituto Nazionale di Fisica della Materia, Universitá di Camerino, I-62032 Camerino, Italy
(Received 11 August 1997)

The unlocking of a linear defect (like a lattice dislocation or a magnetic flux line is a type-II superconductor) from a periodic substrate is modeled by a damped elastic string subjected to a washboard potential. At low temperatures running solutions are shown to set in for tilt amplitudes larger than a certain threshold value, sensitive to the damping constant. Close to the unlocking threshold the motion of a string segment is characterized by a logarithmic transient dynamics; as a consequence, hysteresis effects become observable for forcing periods much longer than any predicted time scale. [S0031-9007(97)04877-1]

PACS numbers: 68.35.Ja, 61.72.Lk, 75.60.Ch

Linear defects in solid state physics are often modeled by a damped elastic string pinned to a periodic substrate potential. Two popular examples are the lattice dislocations in pure crystalline metals [1,2] and the magnetic flux lines through type-II superconducting films [3,4]. In a number of experimental circumstances linear defects are driven by external forces, whence, e.g., the plastic flow of a metallic lattice [5,6] or the dynamical melting of an Abrikosov lattice [7]. The crucial question then arises as how to characterize the steady-state (or *dynamical*) transition between a *locked* phase, where linear defects diffuse thermally on the substrate, and a *running* phase, where, due to inertia, the same defects may be driven over the substrate barriers at the cost of a relatively weak bias [8–11].

The main result of the present Letter is that the threshold value of the driving force at which the dynamical unlocking occurs is determined by the *combined* action of damping and fluctuations. Moreover, in the underdamped limit the unlocking of a string segment is signaled by a logarithmic slowing down of its transient dynamics. Finally, the notion of dynamical unlocking is applied to settle a longstanding controversy about the experimental estimate of an important lattice parameter, the so-called Peierls stress [5].

The *perturbed* sine-Gordon (SG) equation

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

represents the archetypal model of an elastic string at thermal equilibrium on a periodic substrate. The coupling of the classical field $\phi(x,t)$ to the heat bath at temperature T is reproduced here by a viscous term $-\alpha\phi_t$ and a zero-mean Gaussian noise source $\zeta(x,t)$. The damping constant α and the noise intensity are related through the noise autocorrelation function

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

The relevant SG substrate potential $V[\phi] = \omega_0^2(1 - \cos\phi)$ is tilted by the bias term $-F\phi$: the resulting washboard potential retains a multistable structure for $|F| < F_3 \equiv \omega_0^2$ (static unlocking threshold [12]). The elastic string $\phi(x,t)$ can glide perpendicularly to the $V[\phi]$ valleys through two distinct mechanisms:

(a) Thermal nucleation.—A string segment lying along one SG valley, say $\phi(x,0) = 0$, is unstable against the nucleation of thermal kink-antikink pairs [2,6]. Thermal fluctuations, $\zeta(x,t)$ in Eq. (1), trigger the process by activating a critical nucleus. For $F \ll F_3$ an unstable nucleus is well reproduced by the linear superposition of a kink and an antikink, each of size $d = c_0/\omega_0$ and energy $E_0 = 8c_0\omega_0$ [2]. Each nucleus wall experiences two contrasting forces: an attractive force due to the vicinity of the nucleating partner and a repulsive force due to either the uniform force F itself, or the pre-existing (equilibrium) gas of kinks and antikinks [13,14]. On balancing the two forces, one determines the size of the *critical* nucleus, whose energy for $F \ll F_3$ is thus of the order of $2E_0$. At low temperature $kT \ll E_0$ the unlocking time T_N, namely the time a driven string takes to jump out of $\phi(x,0) = 0$, is minimum for $\alpha \ll \omega_0$; according to the transition-state-theory formula [15]

$$T_N = (\pi/\sqrt{2}\,\omega_0)\exp(E_0/kT), \quad (3)$$

(almost) independently of α and F. Hence, a locked string (1) diffuses in the direction of F with exponentially small average speed $2\pi/T_N$.

(b) Running solution.—At vanishingly low temperatures thermal nucleation becomes negligible. The elastic string can still be driven away from a SG valley, say $\phi(x,0) = 0$, provided that the external force F is strong enough. Following [8–10], we assume first that $\zeta(x,t)$ is identically zero and that the intensity F of the driving force increases *adiabatically*. The string will adjust instantaneously around the shifting bottom of its SG valley. Let us define the string mobility μ as

$$\mu(F) = v(F)/F, \quad (4)$$

 0031-9007/97/79(25)/5070(4)$10.00

with $v(F) = \overline{\langle \phi_t(x,t) \rangle}$ and $\langle \phi_t(x,t) \rangle = \lim_{L\to 0} \frac{1}{L} \times \int_0^L \phi_t(x,t)\, dx$. The overbar denotes a suitable time average [16]. It is clear that μ is identically zero (locked solution) as long as F is smaller than the static threshold $F_3 = \omega_0^2$. For $F > F_3$ the string gets unlocked and a free-flow (or running solution) sets in with $v = F/\alpha$ or $\alpha\mu = 1$. Let us now decrease F from $F > F_3$ back to zero. In the inertial regime $\alpha \ll \omega_0$, the string keeps jumping from valley to valley even for $F < F_3$. Such a process comes to a halt only when, at each jump, the potential energy gained by the string gets entirely dissipated by the viscous force $-\alpha\phi_t$. This condition defines the *locking* threshold [12]

$$F_1 = (4/\pi)\alpha\omega_0 = (4/\pi)(\alpha/\omega_0)F_3 . \quad (5)$$

The ensuing hysteresis cycle, illustrated in Fig. 1(a), persists even in the static limit: the string mobility depends on the history of the control parameter F.

However, on setting $\zeta(x,t)$ to zero while keeping the viscous term $-\alpha\phi_t$ in Eq. (1), we have altered the coupling of the SG string to its heat bath. In fact, the fluctuation dissipation relationship (2) required by thermodynamical equilibrium has been violated. In other words, imposing $\zeta(x,t) \equiv 0$ is different from taking the limit $T \to 0$ [17].

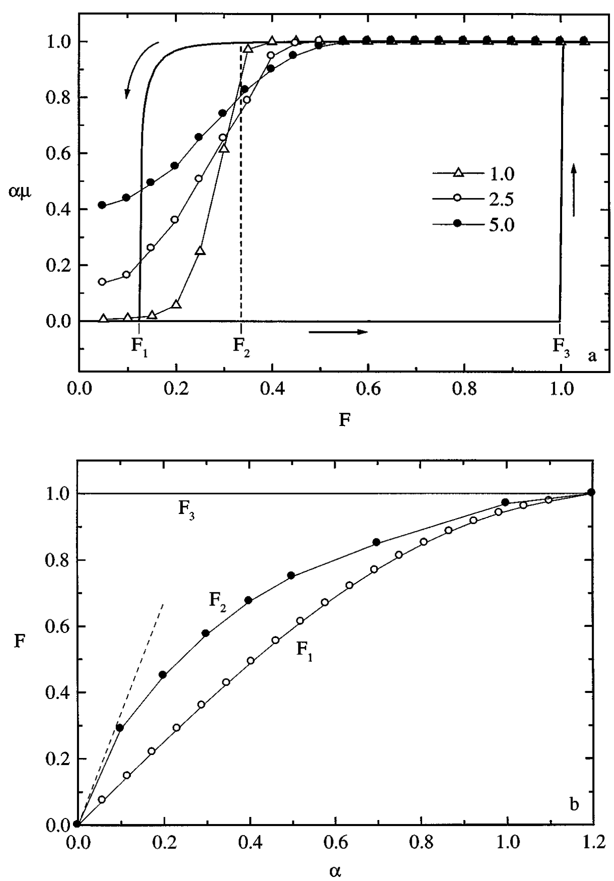

FIG. 1. (a) $\alpha\mu$ versus F for different values of kT. The SG parameters are $\omega_0^2 = 1$, $c_0^2 = 0.1$, $\alpha = 0.1$, and $L = 500$; the integration steps are $\Delta x = 1$ and $\Delta t = 10^{-2}$. The arrows denote the static hysteresis loop discussed in the text. (b) Unlocking thresholds F_1 and F_2 versus α. The dotted line is the analytical prediction (6) for F_2. Here, F_2 is defined as the value of F such that $\alpha\mu = 0.5$ at the lowest temperature in (a), $kT = 1.0$.

In order to clarify this question we ran an extensive digital simulation of Eq. (1) with periodic boundary conditions $\phi(x+L,t) = \phi(x,t)$ and $\phi_x(x+L,t) = \phi_x(x,t)$ and initial conditions $\phi(x,0) = \phi_x(x,0) = 0$. The details of our numerical code and the stability analysis of the resulting string statistics will be reported in a forth-coming article. Here, we limit ourselves to summarizing our main findings. In Fig. 1(a) we plotted the string mobility $\mu(F)$ in the inertial regime $\alpha \ll \omega_0$ at different temperatures [16]. The rescaled mobility $\alpha\mu$ jumps abruptly from marginally small values (due to the nucleation mechanism) up to the (free-flow) asymptotic value $\alpha\mu = 1$ in the vicinity of a new threshold value F_2: such a transition is particularly sharp for T tending to zero, where F_2 can be identified with [18]

$$F_2 \simeq 3.36\alpha\omega_0 = 3.36(\alpha/\omega_0)F_3 , \quad (6)$$

i.e., Risken's threshold for the unlocking of a Brownian particle in a washboard potential [12]. In the *steady-state* regime no hysteresis loop $F_1 \rightleftharpoons F_3$ is observable, at variance with the simulation of Ref. [19]: the dynamical unlocking threshold F_2 turns out to be a uniquely defined function of α. In Fig. 1(b) the two thresholds F_1 and F_2 are plotted against the damping constant: both F_1 and F_2 grow proportional to α for $\alpha \ll \omega_0$ (underdamped limit) and eventually merge together with F_3 for $\alpha > 1.2\omega_0$ (overdamped limit).

The unlocking mechanism of a *string segment* in the presence of thermal fluctuations reveals a number of surprising features which eluded earlier numerical investigations [8,10,19]. In Figs. 2 and 3 we illustrate the transient dynamics of an underdamped SG string at the unlocking threshold F_2. The quantity

$$S(t) = \langle [\phi(x,t) - \langle \phi(x,t) \rangle]^2 \rangle^{1/2} \quad (7)$$

has been introduced in Fig. 2 to describe the diffusion of the string $\phi(x,t)$ around its "center of mass" $\langle \phi(x,t) \rangle = vt$. It is apparent by inspection that: (i) for F close to F_2 the quantity $S(t)$ peaks after a waiting time of the order of T_N, see Eq. (3), thus signaling an unlocking event. The peak of $S(t)$ marks the onset of a running solution with $\alpha\mu = 1$; see Fig. 1; (ii) the decay of $S(t)$ obeys a *logarithmic law* over a time interval τ of up to four decades. In Fig. 2 the transient time τ (independent of L) is of the order of 10^4 to compare with $T_N = 330$; (iii) close to the threshold F_2, the tilt F does control the transient peaks of $S(t)$, but not its asymptotic tails. In fact, trajectories of $S(t)$ obtained for different values of F (above threshold), but *identical* noise sequences, tend to coincide asymptotically—the only difference being a superimposed drift modulation with period $2\pi/v$ [10]

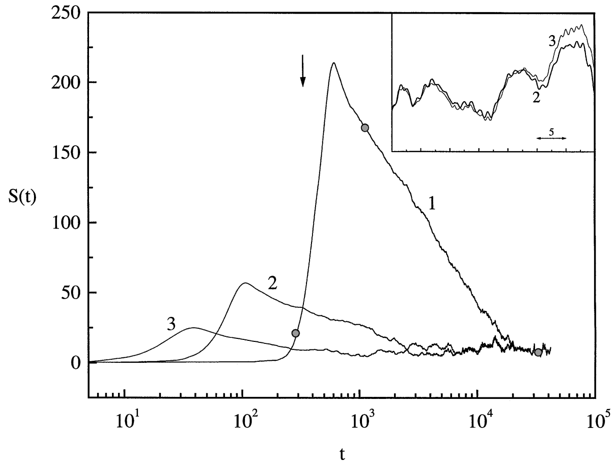

FIG. 2. Transient dynamics: $S(t)$ defined in Eq. (7) versus t for $F = 0.35$ (curve 1), $=0.70$ (curve 2), $=1.0$ (curve 3). The SG parameters are as in Fig. 1 and $kT = 1.0$. The vertical arrow represents the unlocking time T_N of Eq. (3). The three solid circles on curve (1) refer to the string configurations of Fig. 3. Inset: Blowup ($\times 10$) of curves (2) and (3) starting at $t = 1.95 \times 10^4$ (linear scale).

(see inset of Fig. 2); (iv) the unlocking mechanism is triggered by the *nucleation* of multikink avalanches [20] randomly distributed in space and size. The buildup of such avalanches, which may span over many a SG valley, is maximum in correspondence with the rising branch of the $S(t)$ peak and their amplitude s is distributed according to a *power law* $s^{-\delta}$ with $\delta \sim 1$ (see inset of Fig. 3); (v) the string diffusion $S(t)$ attains its peak value $S_{\max} \propto L$ after all avalanches have merged together into a characteristic tonguelike profile as shown in Fig. 3. This property is sensitive to the finite size of the simulated string segment.

The analytical interpretation of the unlocking dynamics is rather involved. First of all, the simulation results of Figs. 1–3 clearly confirm that the string motion can be separated into two components: the drift of the string center of mass $\langle \phi(x,t) \rangle$, which amounts to the Brownian diffusion of an inertial particle in a washboard potential [12], and the spatial diffusion of the string around $\langle \phi(x,t) \rangle$. In the presence of thermal fluctuations the string instabilities detected in Refs. [8–10] disappear: the spatial diffusion of the string builds up through the avalanche mechanism illustrated in Fig. 3 and not as an effect of parametric resonance. After the logarithmic transient is over, the average diffusion $\bar{S} = \lim_{T\to\infty} \frac{1}{T} \int_t^{t+T} S(t')\, dt'$ is well approximated by $\sqrt{kTL/c_0^2/2\pi}$, the average diffusion for a *free* elastic string segment of the same length L and coupled to the same heat bath ($\omega_0 = F = 0$).

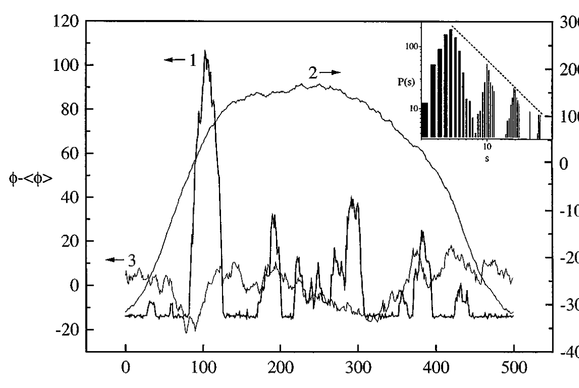

FIG. 3. String segment profiles close to the unlocking threshold ($F = 0.35$) at increasing simulations times ($1 \to 3$). These string configurations refer to the solid circles on curve (1) of Fig. 2. Inset: normalized histogram of the avalanche amplitudes s. The power law $s^{-\delta}$ with $\delta = 1.0$ is drawn for comparison.

The logarithmic decay of $S(t)$ can be explained as follows. The tonguelike profile of $\phi(x,t)$—in coincidence with $S_{\max}$—is made of a large number of kink-antikink pairs subjected to a nonlinear relaxation dynamics. The amplitude $s(t)$ of a large avalanche decays in time due to the viscous damping that opposes the *lateral* motion of each kink (antikink). Therefore, during the transient interval τ, the dominating recovery force acting upon s is proportional to s^2 [14]: in the underdamped limit $\ddot{s} \propto s^2$, whence the logarithmic decay branch of the $S(t)$ peak.

The slow transient dynamics in the vicinity of F_2 makes the nonstationary properties [21] of a driven SG string particularly interesting. In Fig. 4 we display the hysteresis loops we obtained by forcing the SG string with the periodic drive $F(t) = F_0 + F_\Omega \sin(\Omega t)$. Away from the threshold, $F_0 \gg F_2$ or $F_0 \ll F_2$, no hysteresis cycle is detectable for $\Omega T_N \ll 1$, as one would expect for the Brownian motion in a modulated multistable potential

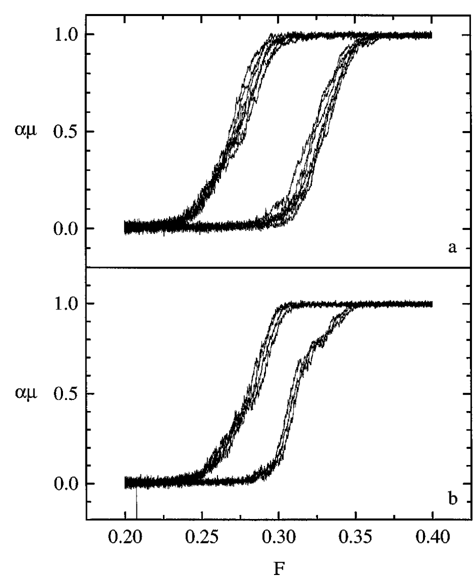

FIG. 4. Hysteresis loops driven by $F(t) = F_0 + F_\Omega \sin(\Omega t)$ with $F_0 = 0.3$, $F_\Omega = 0.1$, and (a) $T_\Omega = 5 \times 10^3$; (b) $T_\Omega = 10^4$. The SG parameters are as in Fig. 1 and $kT = 1.0$.

[22]. At the threshold $F_0 \sim F_2$, instead, hysteresis cycles may be observed for forcing periods $T_\Omega = 2\pi/\Omega$ as large as 10^4, i.e., much larger than T_N (but smaller than τ). This phenomenon is a clear-cut signature of the dynamical unlocking of the string and should not be mistaken for the static hysteresis in the absence of thermal fluctuations $\zeta(x,t) \equiv 0$, mentioned above [10].

The physical implications of the notion of dynamical unlocking may be remarkable, indeed. A possible application is suggested in Ref. [10]. The estimate of the Peierls stress σ_p (which characterizes the amplitude of the substrate modulations in the dislocation glide planes [23]) in fcc metals has been matter for controversy since the early 1950s. The experimental measurements of σ_p may be divided into two classes: (a) *equilibrium* measurements. The internal friction curve of a cold worked metallic sample is drawn as a function of the temperature; the resulting low-temperature peak (the Bordoni peak [6]) is attributed to a mechanism of (unbiased) thermal *nucleation,* so that an experimental value $\sigma_p^{(B)}$ for the Peierls stress can be predicted from the estimated energy $2E_0$ of the relevant critical nucleus [24]; (b) *nonequilibrium* measurements. The low-temperature plasticity threshold σ_f of a metal has been often taken as an alternative, more direct measurement $\sigma_p^{(f)}$ of the Peierls stress, based on the assumption of static unlocking, that is $\sigma_p^{(f)} = \sigma_f$. However, especially for f.c.c. metals, the ratio $\sigma_p^{(f)}/\sigma_p^{(B)}$ turns out to be of the order of 10^{-2} or smaller [5,20]. The explanation of such a discrepancy is surprisingly simple if one notices that the dislocation dynamics on the Peierls substrate of a fcc metal is underdamped [1]. This implies that the plasticity threshold σ_f must be regarded as an experimental measurement of the *dynamical* unlocking threshold F_2 rather than of the static unlocking threshold F_3. In lattice units [23]

$$\sigma_p^{(f)}/\sigma_p^{(B)} = F_2/F_3 = 3.36(\alpha/\omega_0). \tag{8}$$

For commercial pure copper (3-4 N) a reasonable estimate for the damping constant at low temperature $T < 50$ K is $\alpha/\omega_0 \sim (5\text{–}10) \times 10^{-3}$ [1], while a preliminary analysis of the Bordoni peak data yields $\sigma_p^{(B)} = 1.5 \times 10^{-3}G$ [24]. From Eq. (8) we thus predict $\sigma_f = (2\text{–}5) \times 10^{-5}G$ in good agreement with numerous experiments. The long-standing controversy about the Peierls stress estimate is thus settled in terms of the simple model of Eqs. (1) and (2).

Work supported in part by the Istituto Nazionale di Fisica Nucleare (INFN), VIRGO Project. One of the authors (F. M.) wishes to thank D. K. Campbell and A. V. Granato for useful discussions.

[1] A. V. Granato and K. Lücke, in *Physical Acoustics,* edited by W. P. Mason (Academic, New York, 1966), Vol. IVA, p. 225.

[2] J. P. Hirth and J. Lothe, *Theory of Dislocations* (Wiley, New York, 1982), Chap. 8.

[3] G. Blatter *et al.,* Rev. Mod. Phys. **66**, 1125 (1994).

[4] D. R. Nelson and V. M. Vinokur, Phys. Rev. B **48**, 13 060 (1993).

[5] F. R. N. Nabarro, Philos. Mag. A **75**, 703 (1997).

[6] D. H. Niblett, in *Physical Acoustics*, edited by W. P. Mason (Academic, New York, 1966), Vol. IIIA, p. 77.

[7] M. J. Higgins and S. Bhattacharya, Physica (Amsterdam) **257C**, 232 (1996).

[8] S. Watanabe, S. H. Strogatz, H. S. J. van der Zant, and T. P. Orlando, Phys. Rev. Lett. **74**, 379 (1995).

[9] S. Watanabe, H. S. J. van der Zant, S. H. Strogatz, and T. P. Orlando, Physica (Amsterdam) **97D**, 429 (1996).

[10] E. B. Kolomeisky, T. Curcic, and J. P. Straley, Phys. Rev. Lett. **75**, 1775 (1995).

[11] In the present study the effects of spatial disorder on the unlocking mechanism are neglected. See, e.g., V. M. Vinokur, M. C. Marchetti, and L. W. Chen, Phys. Rev. Lett. **77**, 1845 (1996).

[12] H. Risken, *The Fokker-Planck Equation* (Springer, Berlin, 1984), Chap. 11.

[13] P. Hänggi, F. Marchesoni, and P. Sodano, Phys. Rev. Lett. **60**, 2563 (1988).

[14] F. Marchesoni, Phys. Rev. Lett. **73**, 2394 (1994).

[15] P. Hänggi, F. Marchesoni, and P. Riseborough, Europhys. Lett. **13**, 217 (1990).

[16] The periodic components of $\langle\phi(x,t)\rangle$ have been eliminated by further time averaging over the drift modulation period $2\pi/v(F)$.

[17] It would be statistically inconsistent to infer from Eq. (2) that $T \to 0+$ implies $\zeta(x,t) \equiv 0$. In fact, the combined action of fluctuation and dissipation guarantees statistical equilibrium to set in, no matter how low T. On the contrary, damping alone would drive the system toward any of its metastable configurations, depending on the initial conditions. Therefore, when computing zero-temperature equilibrium observables, the limit $T \to 0+$ has to be taken only after the statistical averages have been computed. For a detailed discussion, see, e.g., Ref. [12].

[18] For $L \geq 500$ finite size corrections are negligible. In fact, the maximum speed of a ballistic kink (antikink) is c_0 [2], whence $L/c_0 \gg T_N$. Therefore, unlocking becomes insensitive to the boundary conditions.

[19] O. M. Braun, T. Dauxois, M. V. Paliy, and M. Peyrard, Phys. Rev. E **55**, 3598 (1997).

[20] T. Suzuki and H. Koizumi, Philos. Mag. A **67**, 1153 (1993).

[21] G. Gremaud, M. Bujard, and W. Benoit, J. Appl. Phys. **61**, 1795 (1987).

[22] D. Bose and S. K. Sarkar, Phys. Lett. A **232**, 49 (1997).

[23] To make contact with a real dislocation, lattice units must be restored in Eq. (1), i.e., $\phi \to 2\pi\phi/a$, $c_0^2 \to C/\pi\rho a^2$, $\omega_0^2 \to 2\sigma_p b/\rho a^3$, $\alpha \to B/\pi\rho a^3$, and $F(t) \to 2b\sigma(t)/\rho a^3$, 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 tension constants, G is the shear modulus, and σ_p is the Peierls stress to determine.

[24] F. Marchesoni, Phys. Rev. Lett. **74**, 2973 (1995).