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1989 J. Phys.: Condens. Matter 1 6649

(http://iopscience.iop.org/0953-8984/1/37/012)

J. Phys.: Condens. Matter **1** (1989) 6649–6664. Printed in the UK

Elasticity and the threshold for stress-induced phase-slip in charge-density waves: predictions of a simple model

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Received 15 August 1988, in final form 13 March 1989

Abstract. A simple mean-field model is used to examine the response to stress of the charge-density wave (CDW) in a Peierls–Fröhlich conductor. The strain in the CDW is assumed to be uniform on the scale of the coherence length, and allowance is made for long-range Coulomb interactions, screened by any chains not concerned in the CDW. Details are given of the elastic properties of the CDW both in the linear regime of small strain and in the non-linear case of strain approaching the elastic limit, beyond which the CDW collapses in a process of phase-slip that the model is not adequate to describe. The extent to which the model may describe real CDWs is discussed, with particular reference to the possible relevance of the elastic limit to the threshold field for Fröhlich conduction.

1. Introuduction

In $NbSe_3$, and some other chain-like metallic compounds, the field-induced motion of incommensurate charge-density waves (CDW) gives rise to most unusual electrical properties (see [1] for reviews). The CDW develop, below a critical value T_P of the temperature T, apparently as a result of the Peierls instability [2] of the quasi-low-dimensional electron–lattice system. Their motion, which is associated with a drift of the entire electron distribution and leads to cooperative conduction as proposed by Fröhlich [3], is manifest in non-linear conductivity in steady fields $\mathscr{E}$ stronger than a threshold value $\mathscr{E}_T$, and in numerous switching, hysteresis and memory effects.

The basis of most attempts to account for these phenomena has been the semi-classical phenomenological model of Fukuyama, Lee and Rice (FLR) [4, 5]. This treats the CDW as a continuous, elastically deformable object that 'slides' over a 'pinning' potential, responsible for $\mathscr{E}_T$, due supposedly to randomly distributed impurities.

However, although the features of such motion [6–8] bear a qualitative resemblance to much that is observed, it is obvious that the FLR model cannot apply universally. Inelastic behaviour of the CDW, in processes of phase-slip, is clearly essential to sustained Fröhlich conduction when (as is usual) terminals are arranged so that the continuously moving region of CDW adjoins others that suffer no net translation. Further, it now seems that phase-slip occurs within the moving region itself: there is substantial evidence [9] in support of the view of Tucker *et al* [10] that the pinning is overcome, not by the sliding of the CDW as a continuous body, but rather by the local collapse of its order parameter,

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followed by re-formation with altered phase. Clearly, if phase-slip is necesary for motion to occur, $\mathscr{E}_T$ represents, at least in part, an elastic limit of the CDW.

The literature contains several discussions of the response of CDW to stress. The linear elastic regime, close to equilibrium, has been treated microscopically, most recently by Takada and co-workers [11, 12] in connection with wave-like excitations of the CDW. Most discussion of the non-linear behaviour concerned in phase-slip has been at a phenomenological level, the treatments by Ong and Maki [13] and by Feinberg and Friedel [14] of the generation of phase vortices (dislocations) by non-uniform current flow being examples. Microscopically based analyses of phase-slip are available, however, for two one-dimensional situations, with current density uniform in the transverse direction. The case of a gapless CDW, analogous to a gapless superconductor, is analysed by Batistić *et al* [15] in terms of a time-dependent Landau equation, the parameters of which are justifiable in microscopic terms both in order of magnitude and in their variation with temperature. Of more practical interest is the case of a CDW whose energy gap is not suppressed in equilibrium, to which Artemenko, Volkov and Kruglov (AVK) [16] apply time-dependent Green function techniques developed in connection with non-equilibrium superconductivity.

While such advanced techniques are needed to deal with the dynamics of the phase-slip process, the static problem of finding the threshold for phase-slip to commence can, in certain circumstances, be solved much more simply. The essential requirement is that, below threshold, the strain in the CDW is uniform on the scale of the coherence lengths $\xi_\parallel$ and $\xi_\perp$ in the longitudinal and transverse directions. With the contribution of other derivatives of the order parameter ψ then negligible, the free energy at given T becomes a function only of the strain, from which can be determined the elastic limit beyond which phase-slip becomes inevitable. This treatment in terms of macroscopic elasticity cannot, of course, be extended to the phase-slip process itself, when ψ collapses on a scale of the order of $\xi_\parallel$. It should, however, apply to its onset in those effectively one-dimensional situations where the phase-slip occurs on surfaces, normal to the chains, and having longitudinal separation and transverse dimensions large in comparison respectively with $\xi_\parallel$ and $\xi_\perp$.

Although AVK analyse such a situation, with strain uniform until phase-slip commences, they obtain the elastic limit only as a low-temperature approximation, which proves to require correction when $T > 0$.

In this paper the limit is found by the much simpler method of imposing changes in wavevector on the CDW in a Peierls quasi-one-dimensional metal. The problem can be formulated in terms of the occupation of Bloch states, leading to an elementary microscopic model of CDW elasticity, which nevertheless covers the entire range of temperature, is not limited to the linear regime, and can take account of long-range Coulomb interactions which, as AVK point out, play an essential part in the phase-slip process.

As, despite the simplicity of the model, few quantitative details of its elastic properties are available in the literature, its behaviour up to the elastic limit is examined in some detail. Its possible relevance to experiment is then discussed.

2. Strained CDW in the mean-field approximation

2.1. Basic assumptions

As is usual in mean-field treatments (notably that of Lee, Rice and Anderson [17, 18]), the CDW is assumed to arise from the Peierls instability in a quasi-one-dimensional energy

band, with the lattice replaced by an elastically deformable continuum, and fluctuations (and thus phonons other than in the macroscopically occupied state representing the static Peierls distortion) ignored. Only the long-range effects of Coulomb interactions are taken into account explicitly, through their contribution to the potential energy when distortion of the CDW leads to a departure from charge neutrality on a macroscopic scale. Some allowance for the microscopic effects of Coulomb forces is, however, implicit in the model: electron–electron interactions within chains influence the band structure, and those between chains assist the correlation between their Peierls distortions that mean-field theory assumes.

With these assumptions, the system behaves as one of independent electrons moving in the periodic potential produced by the Peierls distortion. The potential, which will be assumed to vary as $\cos(\boldsymbol{Q}\cdot\boldsymbol{r}+\varphi)$, with $\boldsymbol{Q}$ parallel to the chain axis and φ independent of position $\boldsymbol{r}$, generates an energy gap 2Δ in the electronic energy spectrum.

The single-particle states then have energies

$$E_k = Z_k + (Y_k + \Delta^2)^{1/2} \tag{1a}$$

where

$$\begin{aligned} Z_k &= \tfrac{1}{2}(\varepsilon_k + \varepsilon_{k-Q}) \\ Y_k &= \tfrac{1}{2}(\varepsilon_k - \varepsilon_{k-Q}) \end{aligned} \tag{1b}$$

and ε is the energy in the absence of lattice distortion. Except where noted otherwise, energies will be defined with reference to the band structure, and measured from the Fermi level ε_F of the undistorted system (corresponding to $k = \pm k_F$).

The free energy of the electron–lattice system, per unit volume and at temperature $T = (\beta k_B)^{-1}$, is then

$$F = \tfrac{1}{2}N(\varepsilon_F)\lambda^{-1}\Delta^2 + nE_F - (1/\beta)\sum_k \ln\{1 + \exp[-\beta(E_k - E_F)]\} \tag{2}$$

where n is the electron density (on a scale large compared with $1/Q$) and E_F is the Fermi energy when the Peierls distortion is present; the sum is restricted to $k > 0$ because each k generates two values of E_k. The term in Δ^2 expresses the elastic energy of the Peierls distortion, in terms of a dimensionless electron–phonon coupling parameter λ, and the density of electron states for the undistorted system, $N(\varepsilon)$.

As only a small range of Q close to $2k_F$ is of interest, λ will be regarded as constant, and E_k assumed to vary linearly with k, giving the idealised band structure of figure 1. The approximations are absorbed by setting an appropriate lower limit $-W$ for ε.

Expression (2) can then be written as

$$\begin{aligned} F = \tfrac{1}{2}N\lambda^{-1}\Delta^2 + nE_F - (N/\beta)\int_0^{W+Z} \ln[\{1 + \exp[\beta(E_F - Z - (Y^2 + \Delta^2)^{1/2})]\} \\ \times \{1 + \exp[\beta(E_F - Z + (Y^2 + \Delta^2)^{1/2})]\}]\,\mathrm{d}Y \end{aligned} \tag{3a}$$

$$\begin{aligned} = \tfrac{1}{2}N\lambda^{-1}\Delta^2 + (n - n_0)E_F + \tfrac{1}{2}NZ^2 - NZE_F - (N/\beta)\int_0^{W} \ln[2\{\cosh[\beta(Z - E_F)] \\ + \cosh[\beta(Y^2 + \Delta^2)^{1/2}]\}]\,\mathrm{d}Y \end{aligned} \tag{3b}$$

where $n_0 = NW$ is the electron density before distortion, and it is assumed that $W \gg Z$,

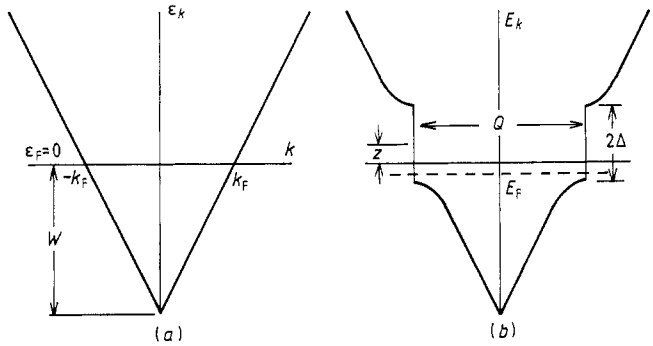

Figure 1. Linearised band structures: (*a*) in the absence of a CDW, and (*b*) with CDW present having $Q > 2k_F$. Energies are measured from the Fermi level ε_F in (*a*). In (*b*), on account of the energy gap at $k = \pm\frac{1}{2}Q$, the Fermi energy is displaced to a new value E_F.

$1/\beta$, Δ. The static behaviour of the CDW is found by minimising F with respect to Δ, subject to such constraints on Q and E_F (or n) as may be appropriate.

2.2 The undistorted CDW

The properties of the model in the absence of constraint on Q are well known, but are repeated here for later reference. In equilibrium one has $Q = 2k_F$ and $n = n_0$, giving $Z = 0$, $E_F = 0$. The free energy

$$F = \tfrac{1}{2}N\lambda^{-1}\Delta^2 - (N/\beta)\int_0^W 2\ln\{2\cosh[\tfrac{1}{2}\beta(Y^2+\Delta^2)^{1/2}]\}\,\mathrm{d}Y \tag{4}$$

is minimised when

$$\int_0^{\frac{1}{2}\beta W} \frac{\tanh[\frac{1}{2}\beta(Y^2+\Delta^2)^{1/2}]}{\frac{1}{2}\beta(Y^2+\Delta^2)^{1/2}}\,\mathrm{d}(\tfrac{1}{2}\beta Y) = 1/\lambda \tag{5}$$

which is the usual BCS-like equation for $\Delta(T)$. The solution at zero temperature is

$$\Delta_0 = 2W\exp(-1/\lambda) \tag{6}$$

and is related to the Peierls temperature T_P by

$$\Delta_0 = \alpha k_B T_P \tag{7}$$

with $\alpha = 1.7639$ ($=\pi\exp(-C)$, $C = 0.5772$ being Euler's constant).

The reduction in free energy due to the formation of the CDW proves, when $T = 0$, to be

$$-\delta F = \tfrac{1}{4}N\Delta_0^2. \tag{8}$$

2.3. Coulomb forces, screening and distortion of CDW

Consider now a steady state of the CDW in which Q, in the presence of pinning and the applied field $\mathscr{E}$, departs from its preferred value $2k_F$. For reasons already given, the strain $(Q - 2k_F)/2k_F$ is assumed uniform on the scale of the longitudinal coherence

length $\xi_{\|} \simeq W/\Delta k_F$. It is also assumed to exist over a length of CDW at least $2\pi/|Q - 2k_F|$, so that the loss or gain of a whole number of wavelengths through phase-slip may reduce the total energy. Although the phase-slip may be induced thermally (and even, in principle, by quantum-mechanical tunnelling), attention is confined here to the case where the CDW collapses because the strain exceeds the elastic limit.

As long as phase continuity is maintained, change in Q implies divergence in the Fröhlich current density. If no electrons were to enter or leave the moving charge distribution, this would cause any departure of Q from equilibrium to be accompanied by a proportionate change in the local electron density n, leaving the Fermi level at the centre of the energy gap, and the magnitude of the gap almost unaffected. In most cases, however, change in n is opposed by Coulomb forces, and reduced also by the maintenance of a unique Fermi energy throughout the crystal. As AVK [16] pointed out, it is the resulting displacement of E_F from the gap centre that causes Δ to diminish, and eventually to collapse, as strain increases.

This effect of strain in reducing Δ is unlikely to be noticeable when the elasticity of a CDW is studied by stressing the crystal as a whole. Strain in the CDW then accompanies identical strain in the lattice to which it is pinned, and bulk neutrality is preserved without E_F being displaced from the gap centre. From expression (3*b*), the increase in free energy associated with strain in the CDW is then $\frac{1}{2}NZ^2$, where $Z = (Q/2k_F - 1)W$. The elastic modulus of the CDW is then $K = (W/Z)\,\mathrm{d}F/\mathrm{d}(Z/W) = n_0 W$, as for a one-dimensional electron gas [4, 19].

The redistribution of electrons, in cases where E_F does leave the gap centre, is popularly said to be effected by 'screening' currents, carried by single particles, as distinct from Fröhlich currents, carried collectively. While the actual transport processes are not of immediate concern, it is noted that this two-fluid view is not adequate to describe the establishment of equilibrium when Z is large, since the number of single particles need not be conserved when Δ and E_F vary. Because of this the term 'screening' is used below in the following restricted sense. Coulomb interactions are said to be unscreened if they prevent the electron density n, on the chains that participate in the CDW, from departing from its undistorted value n_0. For n to differ locally from n_0, the accumulated charge must be compensated by the appearance nearby of an opposite 'screening' charge, minimising the cost in electrostatic energy. Screening charges may appear elsewhere on the CDW chains, or on other chains not concerned in the CDW (and, in principle, on conducting defects within or on the surface of the crystal).

The role of Coulomb interactions in redistributing electrons, with respect to the situation with $n \propto Q$, is apparent from the energy level schemes in figure 2. The undistorted CDW ($Z = 0$) is represented in figure 2(*a*). The situation in a region where $Z > 0$, in the absence of Coulomb interactions, is shown in figure 2(*b*) for the case where no redistribution occurs, and in figure 2(*c*) for the case of equilibrium with a unique Fermi energy E_F (here measured with respect to an external reference) throughout the crystal. Equilibrium in the presence of Coulomb interactions is shown in figure 2(*d*): the band is displaced in energy by an amount $E_c = -eV_c$, where $V_c(\boldsymbol{r})$ is the electrical potential arising from the departure from neutrality, and E_F (now the electrochemical potential) is again uniform throughout the crystal.

Figure 2(*d*) is likely to describe also the local situation in the non-equilibrium steady state reached in an applied field $\mathscr{E} < \mathscr{E}_T$. A single-particle current now flows, but the departure from equilibrium is usually small enough for a (position-dependent) E_F to be defined, with electron temperature unchanged. Further, as the dielectric constant of the crystal will be dominated by the polarisability of the CDW, any accumulation of charge

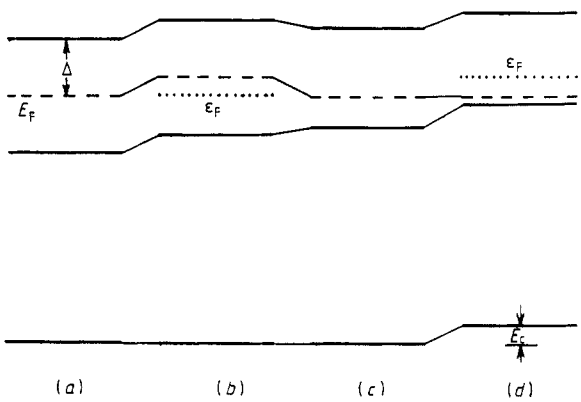

Figure 2. Energy level schemes showing relation of energy gap to Fermi level in distorted CDW. In (*a*) is shown the undistorted CDW; (*b*) the case of $Q > 2k_F$, if no electrons leave the CDW; (*c*) equilibrium in the absence of Coulomb interactions, with Fermi energy unchanged; and (*d*) equilibrium in the presence of Coulomb interactions. The actual Fermi energy E_F is shown as a broken line and the position in the band of the original Fermi energy ε_F as a dotted line. In (*d*) the departure from neutrality causes the band to be displaced in energy by E_c.

not associated with distortion of the CDW may safely be neglected. As its direct contributions to E_F and E_c are equal, the applied field then influences the position of E_F relative to the band structure only through its part in generating the distortion represented by Z.

At any point $\boldsymbol{r}$ the condition of the CDW, when in equilibrium or a steady state as in figure 2(*d*), depends for given $Z(\boldsymbol{r})$ on the local value of $E_c(\boldsymbol{r})$ relative to E_F. As both these depend on Z elsewhere in the crystal (making general solution impracticable), discussion will be of the common situation where $Z(\boldsymbol{r})$ and $E_c(\boldsymbol{r})$ are distributed symmetrically about zero, so that the electrochemical potential has the value that would apply in the absence of distortion. Reverting to the practice of referring electronic energies to the band structure, and measuring with respect to its value ε_F in the absence of distortion, the Fermi energy $E_F(\boldsymbol{r})$ in the strained CDW is then everywhere equal to $-E_c(\boldsymbol{r})$.

A further simplification is made by assuming E_c to be determined by the local value of $n - n_0$; F is then a local function of $Z(\boldsymbol{r})$, and an elastic modulus for the CDW can be defined. This assumption is valid when the screening charges are induced on chains not involved in the CDW (which proves to be the only situation to which the model applies where screening is likely to be appreciable).

In these conditions, the Fermi energy can be expressed as

$$E_F = -E_c = (n - n_0)/NA \tag{9}$$

where A is a screening parameter determined by the geometry; $A = 0$ corresponds to the unscreened case, $A = \infty$ to perfect screening (i.e. negligible Coulomb forces). Adding the appropriate term $\frac{1}{2}(n - n_0)^2/NA$ to expression (3*b*), the free energy density becomes

$$F = \tfrac{1}{2}N\lambda^{-1}\Delta^2 - \tfrac{1}{2}NAE_F + \tfrac{1}{2}NZ^2 - NZE_F - (N/\beta)\int_0^W \ln\left(\frac{\cosh[\beta(Z - E_F)] + \cosh[\beta(Y^2 + \Delta^2)^{1/2}]}{1 + \cosh(\beta Y)}\right) \mathrm{d}Y \tag{10}$$

when measured with respect to the value when $\Delta = 0$. The electron density is related to E_F by

$$n = \sum_k \{\exp[\beta(E_k - E_F)] + 1\}^{-1} \tag{11}$$

which can be expressed as

$$Z + AE_F = \int_0^\infty \frac{\sinh[\beta(Z * E_F)]}{\cosh[\beta(Z - E_F)] + \cosh[\beta(Y^2 + \Delta^2)^{1/2}]}\, dY \tag{12}$$

giving a relation between E_F and Δ. With E_F thus determined, differentiation of (10) with respect to Δ gives

$$\int_0^W \frac{\sinh[\beta(Y^2 + \Delta^2)^{1/2}]}{(Y^2 + \Delta^2)^{1/2}\{\cosh[\beta(Z - E_F)] + \cosh[\beta(Y^2 + \Delta^2)^{1/2}]\}}\, dY = 1/\lambda \tag{13}$$

as the condition for F to be minimum. Solution of the simultaneous equations (12) and (13) then provides Δ, E_F and, from (10), F as functions of the strain parameter Z.

It is then a simple matter to relate the strain Z/W to the stress required to produce it, which can be expressed as

$$\sigma = dF/d(Z/W) = -n_0(1 + A)E_F \tag{14}$$

as may be confirmed by differentiating (10), and using (12) and (13) to eliminate derivatives of E_F and Δ.

3. Elastic properties

3.1. Definitions

It is convenient, in calculating E_F, Δ, F and σ, to introduce units of T_P for temperature, Δ_0 for electron energy, $N\Delta_0^2$ ($= -4\delta F_0$) for free energy density, $n_0\Delta_0$ for stress and n_0W for elastic modulus, with reduced variables defined as follows: $t = T/T_P$, $\delta = \Delta/\Delta_0$, $z = Z/\Delta_0$, $\mu = E_F/\Delta_0$, $y = Y/\Delta_0$, $w = W/\Delta_0$, $f = F/N\Delta_0^2$ and $s = \sigma/n_0\Delta_0$. The reduced elastic modulus $\kappa = K/n_0W$ is then s/z, in the limit $z \to 0$. In terms of these, (10), (12), (13) and (14) become respectively

$$f = \tfrac{1}{2}\delta^2 \ln(2w) - \tfrac{1}{2}A\mu^2 + \tfrac{1}{2}z^2 - z\mu - (t/\alpha)\int_0^w \ln\left(\frac{\cosh[\alpha(z - \mu)/t] + \cosh[\alpha(\delta^2 + y^2)^{1/2}/t]}{1 + \cosh(\alpha y/t)}\right) dy \tag{15}$$

$$z + A\mu = \int_0^\infty \frac{\sinh[\alpha(z - \mu)/t]}{\cosh[\alpha(z - \mu)/t] + \cosh[\alpha(\delta^2 + y^2)^{1/2}/t]}\, dy \tag{16}$$

$$\ln(2w) = \int_0^w \frac{\sinh[\alpha(\delta^2 + y^2)^{1/2}/t]}{(\delta^2 + y^2)^{1/2}\{\cosh[\alpha(z - \mu)/t] + \cosh[\alpha(\delta^2 + y^2)^{1/2}/t]\}}\, dy \tag{17}$$

and

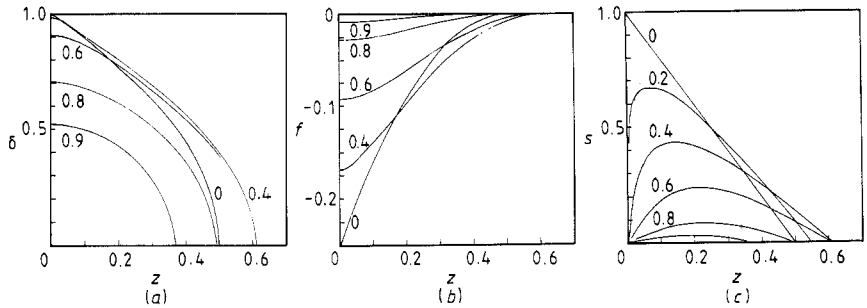

Figure 3. The relation between CDW distortion (represented by the strain parameter z) and (a) energy gap δ, (b) free energy density f, and (c) stress s. The curves refer to the temperatures t indicated. Units are defined in the text.

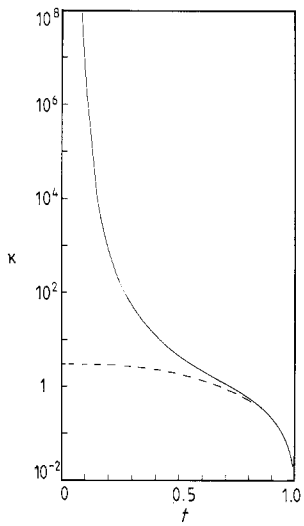

Figure 4. The elastic modulus κ (in units of $n_0 W$) as a function of reduced temperature t. The unscreened case ($A = 0$) is shown by the full curve and an example of partial screening ($A = 0.5$) by the broken curve.

$$s = -(1 + A)\mu \tag{18}$$

where A was defined in § 2.2. Setting $z \ll t$ in (17), one obtains

$$\kappa = (1 - I)(1 + A)/(I + A) \tag{19}$$

where

$$I = \int_0^\infty \frac{\mathrm{d}y}{1 + \cosh[(\alpha\delta/\mathrm{t})^2 + \mathrm{y}^2]^{1/2}}.$$

Except when t is close to 0 or 1, these equations have to be solved numerically (though only for one value of A: a scaling relation connects solutions for different A). The results for the unscreened ($A = 0$) case are given first.

3.2. Elastic behaviour in the absence of screening

Figures 3–5 present the results of solving these equations (by iteration of (16) and (17), giving δ and μ, and thence f and s from (15) and (18)). The CDW exhibits the expected

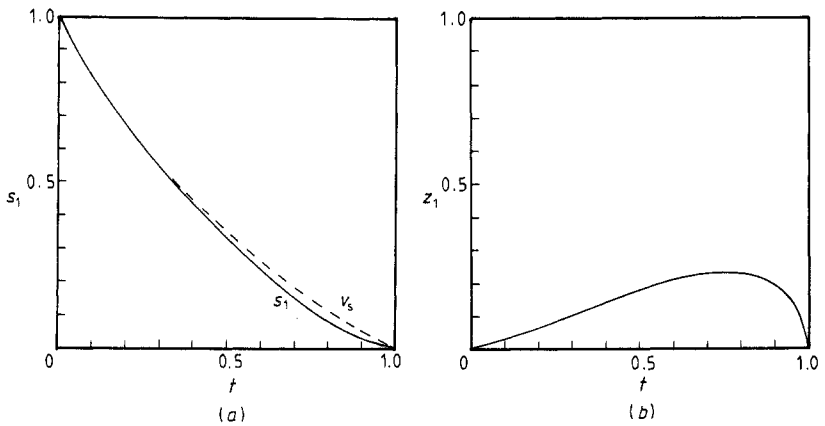

Figure 5. The elastic limit in the unscreened case. Limiting values s_1 of the reduced stress s are shown in (a), and corresponding values z_1 of the strain parameter z in (b), as a function of reduced temperature t. The broken curve in (a) shows the phase-slip voltage V_S, in units of Δ_0/e.

linear elastic response to small z, and eventually collapses when z exceeds an elastic limit.

The reduction of the energy gap δ as the magnitude of the strain parameter z increases is shown in figure 3(a): δ decreases monotonically to zero when z reaches a value z_2, beyond which no CDW is possible. Over most of the temperature range z_2 is close to the value $\frac{1}{2}$, which applies when $t = 0$. The associated increase in the free energy density f is shown in figure 3(b).

The relation between reduced stress s ($= -\mu$) and z is shown in figure 3(c). Except at $t = 0$, $|s|$ at first varies linearly with z, but eventually reaches a limiting value s_1 (when $|z| = z_1$), and thereafter decreases to zero. The situation $s = s_1$, $z = z_1$ represents the elastic limit, beyond which, as $\mathrm{d}s/\mathrm{d}z < 0$, the CDW is unstable with respect to the distribution of strain becoming non-uniform. In the phase-slip that results from this instability, strain becomes concentrated into a length ultimately of the order of $\xi_\parallel$, Δ vanishes locally and the CDW re-forms with reduced distortion. As non-uniformity on the scale of $\xi_\parallel$ is involved, the process, once initiated, lies outside the present treatment.

The reduced elastic modulus κ is shown in figure 4. It rises steadily as t falls, becoming infinite when $t = 0$. Its divergence is a consequence of the unscreened Coulomb interactions (whose part in CDW rigidity was noted by Lee, Rice and Anderson [18]).

The limiting stress s_1 (figure 5(a)) also rises as t falls, but remains finite at $t = 0$. The corresponding limiting strain z_1 (figure 5(b)) necessarily vanishes when $t = 1$, and also when $t = 0$, as the infinite κ/s_1 implies. In effect the CDW, as well as becoming more rigid with decrease in temperature, also becomes stronger but more brittle.

When $t = 0$, the quantities shown in figure 3 become simple functions of z: for positive z, $\delta = (1 - 2z)^{1/2}$, $f = z(1 - z) - \frac{1}{4}$ and $s = -\mu = 1 - 2z$. The linear variation of f, and finite s, for infinitesimal z are symptoms of the rigidity of the CDW when $t = 0$.

When t is slightly greater than 0, κ can be expressed analytically. With $z \ll t \ll 1$, the integral I in (19) approximates to $2(\alpha\delta/t)K_1(\alpha\delta/t)$, where K_1 is the modified Hankel function; κ ($\simeq 1/I$, as $I \ll 1$) is then approximately equal to $\exp(\alpha\delta/t)/(2\pi\alpha\delta/t)^{1/2}$. This result has been obtained, in a different context, by Nakane and Takada [11].

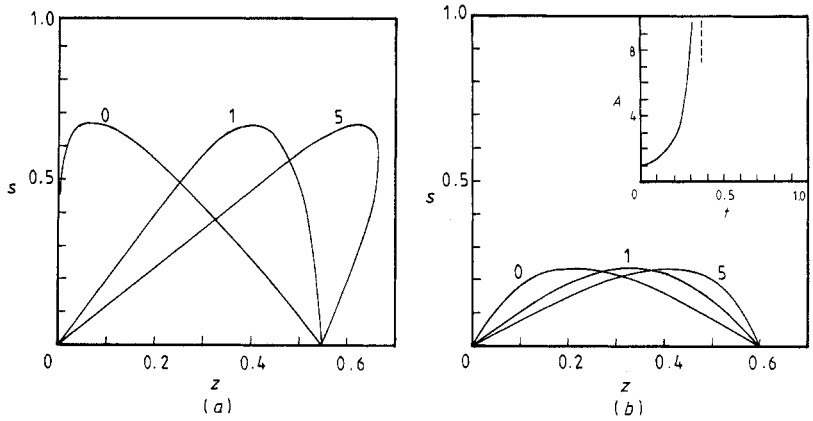

Figure 6. Stress–strain relationships in the presence of screening, shown in (*a*) for reduced temperature $t = 0.2$, and in (*b*) for $t = 0.6$. The curves show (for screening parameter $A = 0$, 1 and 5 as indicated) the relation between strain parameter z and reduced stress s. Metastability is possible when the maximum of s occurs with z greater than the value z_2 for which the CDW vanishes. The graph inset in (*b*) shows, as a function of A, the temperature t_m below which this can happen.

An analytic expression for κ exists also when $t \simeq 1$. With δ then small, and $\alpha\delta/t \ll 1$, $I \simeq 1 - g(\alpha\delta/t)^2$, where $g = 0.2132$ $(=7\zeta(3)/4\pi^2)$, so that $\kappa \simeq g(\alpha\delta/t)^2$. An equivalent result was obtained by Lee, Rice and Anderson [17].

3.3. *The effect of screening*

When $A > 0$, neither δ nor $z + A\mu$ are changed as functions of $z - \mu$ (since A does not appear in (17), or in the integral in (16)). This implies that if the values $z = z_u$ and $\mu = \mu_u$ accompany $\delta = \delta_u$ when $A = 0$, then the values of z and μ that correspond to the same gap δ_u when $A > 0$ are related by $z + A\mu = z_u$ and $z - \mu = z_u - \mu_u$. Thus one has

$$\begin{aligned} \mu &= \mu_u/(1 + A) \\ z &= z_u - \mu_u A/(1 + A) \end{aligned} \tag{20}$$

whence from (18)

$$s = -\mu_u \tag{21}$$

and $\kappa = s/z = (1 - I)(1 + A)/(I + A)$, as already found in (19), since $I \simeq z_u - \mu_u$ when $z_u \ll 1$. As expected, screening eliminates the low-temperature divergence in κ (which now approaches $(1 + 1/A)$ as $t \to 0$), but has little effect when $t \simeq 1$, since then $I \simeq 1$.

The effect on the stress–strain relation is shown in figure 6. The screening, although it reduces κ, has no effect on the limiting stress s_1, as (21) shows. However, the corresponding strain z_1 is increased and may, with A sufficiently large and t small, exceed the strain z_2 at which the CDW eventually vanishes. Such metastability of the CDW is possible (as is evident from (20)) only when $z_{1u} - \mu_{1u}A/(1 + A) > z_2$, where z_{1u} is the value of z_1 when $A = 0$ and μ_{1u} is the corresponding value of μ. This condition can be satisfied if $A > 1$, and then only below a critical temperature t_m, whose dependence on A is shown (inset) in figure 6.

3.4. Coupling to the applied field

The stress σ arises usually from the force that the applied field $\mathscr{E}$ exerts on the CDW between sites of phase-slip. This force can be expressed (per unit volume) as $F_e = -ne\rho_c$, where $\rho_c(t, z)$, the fraction of electrons effectively concerned in the CDW, was defined by Lee and Rice [5]. As an alternative to their method of first finding the force communicated to the single particles, ρ_c can be obtained directly from the rate at which momentum is transferred from them to the Peierls distortion. This rate of transfer is approximately

$$F_e = -\sum_k m\dot{v} \tag{22}$$

where m is the free-electron mass, $\dot{v} = (-e\mathscr{E}/\hbar^2)\partial^2 E_k/\partial k^2$ is the acceleration of an electron in a state k close to the CDW energy gap and the sum is taken over occupied states. This expression intentionally ignores scattering, which transfers momentum to phonons or defects, and any band curvature not associated with the Peierls gap (and not shown in figure 1), which represents transfer from $\mathscr{E}$ to the electrons, and from them directly to the lattice. With E_k as in (1), and the idealised band structure, one has

$$m\dot{v} = \pm e\mathscr{E}W\Delta^2/(Y^2 + \Delta^2)^{3/2} \tag{23}$$

from which, in terms of reduced variables,

$$\rho_c = \delta^2 \int_0^\infty \frac{\sinh[\alpha(y^2 + \delta^2)^{1/2}/t]}{(y^2 + \delta^2)^{3/2}\{\cosh[\alpha(z - \mu)/t] + \cosh[\alpha(y^2 + \delta^2)/t]\}}\,dy \tag{24}$$

where, as previously, $W \gg Z$, $1/\beta$, Δ; a Fermi distribution, implying strong scattering of single electrons, coupled negligibly to phasons, is assumed.

In the elastic range $z < z_1$, ρ_c proves to be slightly greater than the reduced gap δ (by no more than 3% when $t < 0.5$, 13% when $t = 0.9$, and 38% when $t \simeq 1$). As ρ_c is a function of $z - \mu$, screening can again be taken into account by scaling, as in (20).

As $F_e = d\sigma/dx$, with x measured along the CDW, a field $\mathscr{E}$ acting on a length $2L$ of CDW, pinned at its ends, causes the limiting stress s_1 to be reached at the ends when

$$V_s = \mathscr{E}L = (\Delta_0/e)\int_0^{s_1} ds/\rho_c \tag{25}$$

giving the critical voltage V_s associated with phase-slip at a single site. When $t = 0$ this is equal to Δ_0/e. The broken curve in figure 5(*a*) shows its behaviour at other temperatures: V_s is proportional to s_1 when t is small, but when $t \simeq 1$ (where ρ_c varies as $(1 - t)^{1/2}$) it becomes proportional to $(1 - t)$, whereas s_1 varies as $(1 - t)^{3/2}$.

4. Comment

4.1. Applicability

The ability of the model to describe real CDW is limited by its use of mean-field theory in a one-dimensional situation, and by the assumption that the free energy of the CDW depends only on the periodicity Q.

That mean-field theory appears to describe CDW in quasi-low-dimensional metals adequately is presumably a result of the inter-chain correlation provided by Coulomb coupling. Although not expressed by the one-dimensional band structure (the parallel

planes of Fermi surface are spanned by Q having arbitrary component transverse to the chain direction), this coupling provides the CDW with shear strength, so that a unique Peierls distortion, with negligible fluctuations, is possible.

The extension of the model to include shear is elementary: the shear adds to the free energy and so tends to reduce δ, but, as the relevant correlation length $\xi_\perp$ is of the same order as the separation between chains, is not likely to be the immediate cause of collapse in the CDW. Phase-slip may still be regarded essentially as the result of longitudinal stress, with the shear strength limiting the extent to which that stress can be conveyed laterally.

The assumption that Q determines the free energy of the CDW is a more serious limitation. However, although this makes the model incapable of dealing with the actual process of phase-slip, it need not prevent it from specifying the condition for phase-slip to commence.

Clearly, the use of Q to define the state of the static CDW is legitimate only to the extent that the band structure of figure 1(b) is not invalidated by indeterminacy in the electronic wavevectors $\boldsymbol{k}$. Although such indeterminacy may arise from the direct influence on the electronic Bloch states of the obstacles to CDW motion, the range over which those states are modified is small ($\sim k_F^{-1}$) in comparison with $\xi_\parallel$. As far as the elastic behaviour of the CDW is concerned, the result is merely to increase the effective size of the obstacle.

The indeterminacy in $\boldsymbol{k}$, which limits the validity of the model, is, as mentioned at the outset, that arising from non-uniform spatial variation in Q. It is evident from § 3 that this restricts the use of the elastic limit there derived to situations where strain is uniform on a scale $\xi_\parallel/z_1$. This condition is not difficult to satisfy in one-dimensional situations (where it requires the separation of the obstacles at which phase-slip occurs to be large compared with $\xi_\parallel/z_1$), but is more restrictive in three dimensions, where the obstacles have to be large in comparison with $\xi_\parallel/z_1$ and $\xi_\perp/z_1$ respectively in the longitudinal and transverse directions. Close to smaller obstacles the strain is significantly non-uniform, and the elastic limit provides merely a necessary condition for phase-slip (i.e. that the strain should exceed the limit locally) and a sufficient condition (that the limit is exceeded over a length $\xi_\parallel/z_1$).

4.2. *Orders of magnitude*

As a guide to orders of magnitude, a representative (but hypothetical) CDW will be considered, having $T_P = 100$ K, $n_0 = 10^{21}$ cm^{-3}, $Q = 5 \times 10^7$ cm^{-1} and $W = 1.6 \times 10^{-19}$ J = 1 eV. The units defined in § 3 are then: for electron energy, $\Delta_0 = 2.4 \times 10^{-21}$ J (15 meV); free energy density, $N\Delta_0^2 = 0.036$ J cm^{-3}; stress, $n_0\Delta_0 = 2.4$ J cm^{-3}; and elastic modulus, $n_0W = 160$ J cm^{-3}. The longitudinal coherence length $\xi_\parallel$ is about 300 Å when $t = 0$.

The screening parameter A is defined as $-(n - n_0)/NeV_c$, where $N = n_0W$ and V_c is the electrical potential that the electrons on the CDW chains experience when n departs from the original value n_0. Apart from a geometrical factor of the order of unity, V_c can be expressed (in SI units) as $-e(n - n_0)d^2/\varepsilon_0$, where d is some average separation between the charge associated with $(n - n_0)$ and the induced screening charge. Thus $A \simeq (\varepsilon_0/e^2)(W/n_0d^2)$, or $5.5/d^2$ when d is measured in ångströms, with W and n_0 as above.

Evidently screening, in the present sense, is negligible unless it occurs on a microscopic scale, with d of the same order as atomic separations. Such screening is possible in $NbSe_3$, and in monoclinic TaS_3 above 160 K, in which other conducting chains lie

between those on which the CDW forms. For these materials, values of $A \sim 0.5$ appear possible. In other known CDW conductors A should be practically zero, allowing no macroscopic departure of the CDW chains from neutrality, even on the scale of $\xi_{\|}$.

The unscreened elastic modulus (given by figure 4, in units of 160 J cm^{-3}) is about 800 J cm^{-3} when $t = 0.5$, and nearly 10^4 J cm^{-3} when $t = 0.3$. Screening with $A = 0.5$ limits K to 480 J cm^{-3}, even when $t = 0$. Figure 5(*a*) gives the limiting stress s_1 and equivalent voltage V_S (both independent of screening) in units respectively of 2.4 J cm^{-3} and 15 mV. The limiting strain in the unscreened case is available from figure 5(*b*): the maximum at $t \simeq 0.75$ corresponds, with present values of W and Δ_0, to strain $Q/2k_F^{-1}$ $(=z\Delta_0/W)$ approximately 3.5×10^{-3}. In the presence of screening with $A = 0.5$, the maximum strain is sightly larger (4.4×10^{-3}), and occurs at a lower temperature ($t \simeq 0.55$).

4.3. *Comparison with experiment*

The experimental evidence that CDW behave in this way, at least in order of magnitude, is suggestive rather than conclusive, partly because many properties cannot easily be measured directly.

4.3.1. Elastic modulus. Except for those in which the CDW and lattice are strained together, no unambiguous measurements of elastic modulus in CDW have been made. Values of the order predicted above were suggested by early measurements of memory phenomena in $NbSe_3$ [20], but are now suspect, in view of concentration of distortion near current terminals mentioned below. Evidence of the low-temperature rigidity of unscreened CDW has been provided, however, by the recent observation of Fröhlich conduction free of dissipation, except for that incurred in overcoming the threshold field $\mathscr{E}_T$ [21].

4.3.2. Limiting stress, and voltage inducing phase-slip. Where voltages associated with phase-slip have been measured, in short specimens whose behaviour is dominated by processes at current terminals, they have proved to be an order of magnitude smaller than the V_S just predicted, while showing roughly the same dependence on temperature.

One known cause of discrepancy is that phase-slip can be induced thermally, before the limiting stress is reached. This has been shown to happen, at temperatures above $0.5T_P$, in $NbSe_3$ [22] and *o*-TaS_3 [23], and leads to an ill-defined threshold field. However, even where the process is athermal, the applied voltage necessary to induce phase-slip will be smaller than V_s when, as is usual, stress is concentrated by the use of terminals on the side of the crystal.

The resemblance between the behaviour of V_s in figure 5(*a*), and the almost universal tendency of the well defined (and presumably athermal) threshold fields $\mathscr{E}_T$ in bulk material to increase at low temperatures, suggests that stress-induced phase-slip is involved there also. Thresholds of the magnitude observed (0.01–1 V cm^{-1}), together with the observation that the moving CDW retains phase coherence over macroscopic distances, are consistent with phase-slip at obstacles extending over only part of the crystal cross section, with stress concentrated in their vicinity. With n_p such obstacles per unit volume, each having effective area S ($\gg\xi_\perp^2$) normal to the chains, the present model gives $\mathscr{E}_T = 2V_s n_p S$; $\mathscr{E}_T \sim 0.01$ V cm^{-1} might correspond, for example, to $n_p = 5 \times 10^{11}$ cm^{-3}, $S = (100\ \text{Å})^2$.

If $\mathscr{E}_T$ indeed represents the threshold for phase-slip, its rapid increase as T approaches T_P is in apparent conflict with the behaviour of V_s. A possible explanation, due to Lee and Rice [5], is that close to pinning centres T_P (and thus Δ and s_1) is enhanced, while the effective value of ρ_c vanishes at the somewhat lower T_P that applies elsewhere.

4.3.3. Strain. Attempts to measure the longitudinal strain in CDW, using x-ray diffraction, have produced only negative results [24–26], though shearing has been detected [26]. This is not unexpected, in view of the small limiting strain that the model predicts.

Less easy to reconcile with the model is the electrical memory phenomenon known as the 'overshoot' or 'pulse-sign memory' effect, in which a field-induced distortion of the CDW is preserved by pinning. In the case of the higher-temperature CDW in $NbSe_3$ the distortion, which has been found to be concentrated near current terminals and may also include shear, appears to involve longitudinal strains much larger than the limiting values predicted above [22]. This, it has been suggested [14], probably indicates the presence of dislocations.

4.3.4. The metastable state associated with screening. The estimate in §4.2 makes it doubtful whether any material provides enough screening ($A > 1$) support the low-temperature metastable state suggested by § 3.3. Neither is it obvious how that state could be distinguished experimentally from the other metastable states, common in pinned CDW, whose relaxation often leads to detectable changes in single-particle transport properties. Of the many observations of such relaxation, those on $NbSe_3$ at temperatures below 4.2 K ($t < 0.07$) [27] seem the most likely to be of the state in question.

4.3.5. Application to the FLR model of pinning. Caution is necessary in applying the results derived above in conventional (FLR) treatments of pinning. In the case of strong pinning, and when screening is absent, the mean value of the strain introduced by fixing the phase of the CDW at points separated by a distance L, which may amount to π/QL, inevitably exceeds the elastic limit $z_1\Delta_0/W$ predicted by the model as $T \to 0$. However, the restriction to a length L then introduces enough uncertainty into Q to invalidate the model, so that at low temperatures the problem requires microscopic treatment.

With weak pinning the limitations of the model are less apparent. The scale L on which strain is effectively uniform is now the Lee–Rice length, measured in the chain direction. This is proportional to $K_\parallel K_\perp/n_i$, where n_i is the concentration of pinning centres and $K_\parallel$, $K_\perp$ are elastic moduli parallel and perpendicular to the chain direction. At low temperatures $K_\perp$ is likely to be roughly constant, so that $L \propto K_\parallel/n_i$. Provided that n_i is not too large, π/QL then remains less than $z_1\Delta_0/W$ ($\propto 1/K$) as $T \to 0$, and the use for $K_\parallel$ of the macroscopic elastic modulus K given by the model would seem to be justified.

4.3.6. Transport properties. Finally, the role of screening in the dynamics of CDW deserves mention. On account of pinning, motion of CDW involves the establishment of strain, in the course of which electrons have to be transferred from regions in which $Q > 2k_F$ to others where $Q < 2k_F$. It is usual to assume that the transfer is of single particles already excited across the CDW gap, and, in materials that become insulators as $T \to 0$, an observed increase in the viscosity of the CDW at low temperatures has been accounted for qualitatively as a result of the decrease in conductivity due to such particles [28]. Quantitatively, however, the resistance of the CDW to changes in strain is greater than

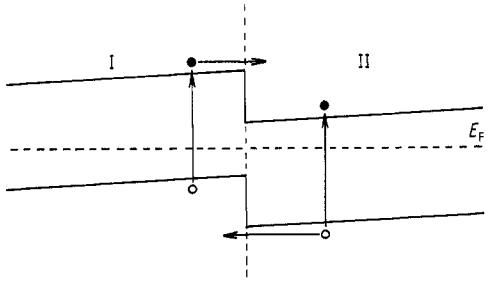

Figure 7. Thermally activated processes involved in the isothermal distortion of a CDW at an obstacle. Each process transfers an electron from the region where $Q > 2k_F(\mathrm{I})$, to that where $Q < 2k_F(\mathrm{II})$. The circles denote electrons (●) and holes (○).

expected, on the basis of reasonable assumptions regarding the distance over which the electrons move.

It is suggested that the discrepancy arises because the maintenance of neutrality requires electrons to be excited thermally across the CDW energy gap. As the transfer of single particles alone, even if sufficient to restore neutrality, would leave the system thermally out of equilibrium, such transitions are essential to the establishment under stress of a state of minimum free energy.

Examples of transitions associated with distortion of a CDW at an obstacle are shown in figure 7. An increase in the distortion, transferring electrons from region I (where $Q > 2k_F$) to region II ($Q < 2k_F$), cannot be accomplished isothermally without excitation across the energy gap. At low temperatures the viscosity of the CDW, while showing activated behaviour qualitatively similar to that of the resistivity when the CDW is undistorted, is likely to be much greater (and to exhibit a somewhat larger activation energy) than the resistivity would suggest.

The difficulty of transferring electrons between strained regions of the CDW at low temperatures also has the effect of postponing the occurrence of phase-slip when a voltage in excess of V_s is applied to an initially undistorted CDW. This may conceivably be relevant to the delayed onset of Fröhlich conduction in 'switching' specimens [29].

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