PHASE STRAIN MODEL FOR CHARGE DENSITY WAVE SUB-DOMAIN FORMATION IN AN APPLIED TEMPERATURE GRADIENT

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The dynamics of a sliding charge density wave (CDW) condensate subjected to a uniform temperature gradient are examined within an elastic medium model. As the temperature gradient is increased, it becomes energetically favorable for the CDW to break up into a series of velocity sub-domains of equal size separated by phase slip centers. The number of sub-domains scales with the temperature gradient and with the length of the CDW crystal. Unusual dynamical asymmetries are also predicted depending on the relative direction of heat and current flow through the CDW crystal.

One of the most intriguing aspects of the collective mode charge density wave (CDW) state is that it exhibits long-range phase coherence. For a dynamic (that is, "sliding") CDW condensate, the phase velocity coherence length is a macroscopic quantity. In materials such as NbSe$_3$, TaS$_3$, and K$_2$MoO$_3$, the characteristic parameters dictating the CDW response (such as normal-carrier damping, number of carriers in the CDW state, threshold electric field $E_T$, etc.) are, in general, very temperature dependent. Hence, for a given external drive condition (electric field or current), the CDW response (namely, the CDW drift velocity $v_0$) is temperature dependent.

For a sliding CDW crystal subject to a temperature gradient along the crystal axis, there exists a competition between the tendency for macroscopic CDW phase coherence and the tendency for the CDW velocity to assume a distribution of values dictated by local conditions. Indeed, early narrow-band "noise" (NBN) experiments (where the well-defined noise frequency $f_{NBN}$ gives directly $v_0$) on NbSe$_3$ samples subjected to a temperature gradient have shown that for very short crystals, $v_0$ is single valued and reflects only the average sample temperature while, for longer samples, the single velocity "domain" (apparent under isothermal conditions) breaks into two or more "sub-domains" with independent $v_0$'s. Thus, under appropriate conditions, an applied temperature gradient is able to break the CDW coherence and induce sub-domain formation.

In this report, we examine within a simplified model the competition between macroscopic CDW phase coherence and velocity sub-domain formation in a CDW crystal with an applied uniform temperature gradient. We model the CDW as an elastic medium subject to internal temperature-gradient-induced strain where excessive strain is relieved by the formation of velocity sub-domains separated by phase slip centers (PSC). From a general energy minimization scheme, we find that in the high field limit ($E>>E_T$) the sub-domains are of equal size and that the number of sub-domains $N$ scales directly with the temperature difference $\Delta T$ across the sample and with the length $L$ of the sample: $N \sim \Delta T^{2/3} L^{1/3}$ in one limit, and $N \sim \Delta T^{2/5} L^{3/5}$ in another limit. This prediction has, in part, been verified by recent experiments in NbSe$_3$. In addition, for a given sub-domain, the model predicts asymmetries in $v_0$ with respect to the relative directions of heat and current flow through the crystal. This $v_0$ asymmetry may explain previously observed but poorly understood differences between noise spectra for positive and negative drive in CDW crystals.

We represent the charge density by the usual expression $\rho(x) = \rho_0 + \rho_1 \cos[qx + \Phi(x,t)]$ where $\rho_0$ is the mean electronic charge density, $\rho_1$ is the density wave amplitude, $q = 2k_F$ is the CDW wavevector, and $\Phi(x,t)$ is the position and time dependent CDW phase whose time derivative is related to the CDW velocity $v_0$. To conform with experimental observations, we assume that, with the application of a temperature difference $\Delta T$ across the crystal, the sample breaks into $N$ sub-domains and that the CDW velocity $v_0$ is constant only over a particular sub-domain. Thus, for a given sub-domain, $\Phi(x,t) = Q_0 v_0 t + \Phi(x)$ where $\Phi(x)$ is a (time independent) distortion. The coordinate $x = 0$ is here defined to lie in the center of the sub-domain.

Due to the temperature variation across the sub-domain, the moving CDW will generate a position-dependent internal elastic strain $s$ which, in turn, leads to position dependences in the CDW wavevector, charge density, and damping. The internal strain is parameterized by $s = s(x) \equiv (1/Q) d\Phi(x)/dx = \Delta Q/Q$. Within a sub-domain, the CDW equation of motion is taken as:

$$\frac{d^2 \Phi(x)}{dt^2} - \frac{1}{Q} \frac{dQ}{dx} \left( \frac{d\Phi(x)}{dx} \right) = \rho_0(x) E(x)$$

where $\gamma$ and $\kappa$ are, respectively, the CDW damping and elasticity. To first order, the position dependences of $\kappa$ and the applied electric field $E$ result from the temperature variation $T(x)$ while the position dependence of $\rho_0$ is...
dominated by the strain $\rho_0(x) = \rho_0 - \rho_s$, and the damping has strain and temperature terms $(\gamma(x) = \gamma + \gamma'\Delta T/Lx - \gamma_0)$. The high-field limit is assumed which eliminates the threshold field. In the limit of small $\Delta T$, Eq. (1) leads to a sub-domain phase velocity

$$v_0 = \frac{\rho_0 E}{\gamma} \delta \left[ \frac{1}{2} \frac{L_0 E^2 \Delta T}{2\varepsilon L} \frac{\xi(E)}{\varepsilon} \right]$$

(2a)

where $p = (\rho_0 y)/(\rho_s)$ and the primes denote temperature derivatives. The associated sub-domain strain $s(x)$ derived from Eq. (1) is

$$s(x) = \coth(v) \cdot \frac{1}{v}$$

(2b)

$$\frac{E}{\varepsilon} = \alpha \frac{L_0}{2} = \frac{\rho_0 E L_0}{2\kappa} (1 - r)$$

(2c)

Far from the transition temperature, these parameters are not very temperature dependent so we treat $U_{ps}$ as being a constant independent of temperature and position.

For $N$ sub-domains, the total energy becomes

$$U_{tot} = U_{ps}(N + 1) + U_{ps}$$

(4)

where we have defined the total strain energy $U_{ps} = \sum U_{si}$. The position of the sub-domain interfaces (which, in turn, dictates the individual sub-domain sizes $L_{Di}$) are found by minimizing, for a given $N$, the total strain energy $U_{si}$. With $p_i$, the position of the $i$th phase slip interface, the appropriate minimization condition is

$$\frac{dU_{si}(L_{Di})}{dL_{Di}} = 0, 1 \leq i \leq N - 1,$$

which has the solution $L_{Di} = L/N$, that is, all the sub-domains are of equal size. With this assignment, Eq. (4) leads to

$$U_{tot} = \frac{U_{ps}(N + 1) + \frac{B_m(\Delta T)^2 L^{m-2}}{N^{m-1}}}{N^{m-1}}$$

(5)

where $B_m$ is a weak function (and can be taken as a constant) whose limiting form depends on $bol$, and $m = 3$ in the large-$bol$ limit and $m = 5$ in the small-$bol$ limit. The second term on the right in Eq. (5) is $U_{si} = U_{bol}/N^{m-1}$. The critical value at $\Delta T$ at which the total number of sub-domains in the crystal will change by one is determined from Eq. (5) by setting $U_{tot} = \frac{U_{bol}}{N^{m-1}}$. This leads to

$$U_{Tol,N} = U_{ps}(N - 1) + \frac{B_m(\Delta T)^2 L^{m-2}}{N^{m-1}}$$

(6a)

$$U_{Tol,N} = \frac{N^2 (N + 1)^2}{2N + 1}$$

(large $|\nu|$)

(6b)

$$U_{Tol,N} = \frac{4N^2 (N + 1)^4}{4N^3 - 6N^2 + 3N + 1}$$

(small $|\nu|$)

Figure 2 shows the total number of sub-domains $N$ plotted versus the normalized strain energy $U_{tot}/U_{ps}$, appropriate to the large-$bol$ limit. In the limit of large $N$, the
Fig. 2. Number of sub-domains \( N \) versus normalized strain energy \( U_s/U_{ps} \) calculated in the large-\( \alpha \) regime (Eq. (6a)). The approximate expression for \( N \) (Eq. (7a)) is also plotted for comparison (solid line). The inset shows in detail \( N \) for small strain energy.

The number of sub-domains can be written in closed form:

\[
N = \left( \frac{2U_s}{U_{ps}} \right)^{1/3} = \left( \frac{2B_m|\Delta T|^2 L}{U_{ps}} \right)^{1/3} \quad \text{(large } |v| \text{)} \quad (7a)
\]

\[
N = \left( \frac{4U_s}{U_{ps}} \right)^{1/5} = \left( \frac{2B_mE^2|\Delta T|^2 L}{U_{ps}} \right)^{1/5} \quad \text{(small } |v| \text{)} \quad (7b)
\]

which demonstrates directly a surprising scaling between \( N \) and \( \Delta T \) for fixed \( L \) and between \( N \) and \( L \) for fixed \( \Delta T \). The solid line in Fig. 2 is Eq. (7a) which compares favorably with the numerical solution even in the range of small \( N \) (see inset).

Recent experiments on NbSe\(_3\) have carefully examined the relation between the sub-domain number \( N \) and the applied temperature gradient \( \Delta T \). The relation \( N \sim (\Delta T)^{2.5} \) is accurately obeyed for several NbSe\(_3\) specimens over a wide range of \( \Delta T \) for both positive and negative values of \( \Delta T \). This scaling behavior is consistent with Eq. (7a) and suggests that typical samples of this material fall into the large-\( \alpha \) limit. For \( N = 4 \) or 5, the relative energy scale is \( U_{ps} / U_{ps} \sim 50 \). The scaling relation of \( N \) versus sample length \( L \) has not yet been tested.

We also note that Eq. (2), the expression for the CDW velocity \( v_0 \) within a sub-domain, has an unusual asymmetry with respect to the signs of \( E \) and \( \Delta T \). If both \( \Delta T \) and \( E \) are reversed, the equation remains invariant. On the other hand, if only \( \Delta T \) or only \( E \) is reversed in sign, the expression for \( v_0 \) is markedly different. The magnitude of \( v_0 \) plays an essential role in determining \( N \) in Eq. (6). Hence, in the presence of a fixed-temperature gradient, the model suggests that a different number of sub-domains can result depending on the relative directions of the electrical and heat currents in the sample. This has been observed experimentally in NbSe\(_3\). Furthermore, this phenomenon may be the cause of asymmetries observed in the noise spectra of CDW conductors under isothermal conditions. In those cases, an inhomogeneous impurity distribution may manifest itself as (very loosely speaking) a "built-in" temperature gradient (that is, a built-in strain asymmetry) with the consequent difference in domain configuration or magnitude of \( v_0 \) for positive and negative drive bias.

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References

8. P. A. Parilla, M. F. Hundley, and A. Zettl, to be published.
10. Actually, \( U_S \) is a more complicated function of the \( \rho_i \) than just the \( L/X \) dependence; however, the \( L/X \) dependence strongly dominates. (see Ref. 8)