HYDRODYNAMICS OF PLASTIC FLOWS WITH CURRENT CONVERSION

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Outline

- Electronic crystals.
- Experiments on pastic flows and current conversion
- Two types of dislocation motion
- Kinematics at presence of dislocation lines/loops, invariant averaging.
- From kinematics to dynamics. Materials relations and kinetics.
- Where does the stress in density waves come from.
- 1D regime, electric field actions, correlation between stress and chemical potential.
- Conclusions

Main features of electronic crystals

- Periodicity follows a local concentration of electrons
- Crystal is sliding as a whole under the driving field above the threshold E_t.
- Collective sliding is a periodic highly coherent but strongly anharmonic process.
- Excess normal current is converted to the collective one via phase slip processes.
- Point defects, vacancies are favorable in compare to electrons as normal carriers.
- Perpendicular flow of dislocations is an ingredient of the sliding and of the current conversion.
- **CDW/SDW specifics:** the energetics of dislocation lines/loops is determined by the Coulomb forces and by screening facilities of the free carriers.

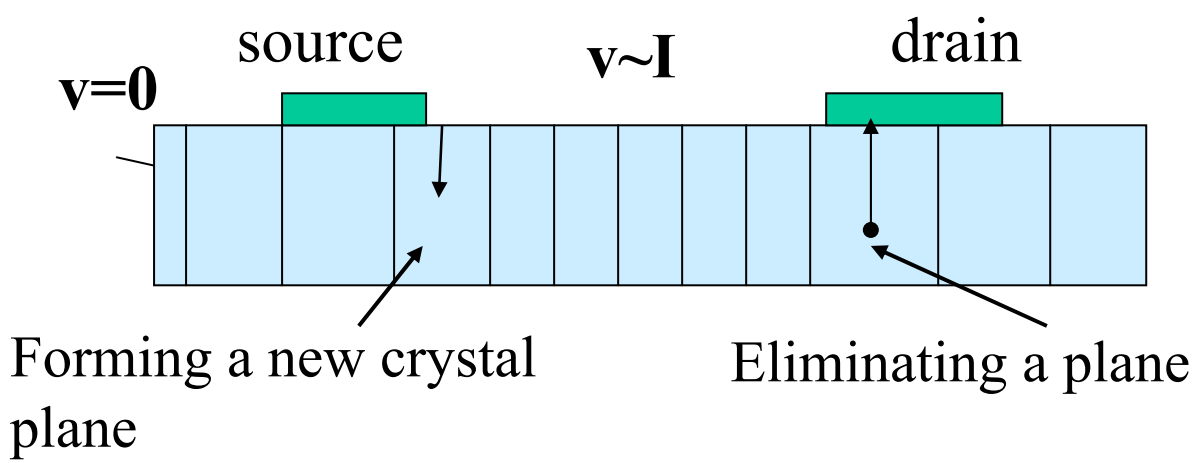
Topological defects in electronic crystals: CDW, SDW

Solitons, phase slips and dislocation lines/loops

Phase slips:

Microscopically – selftrapping of electrons into solitons with their subsequent aggregation

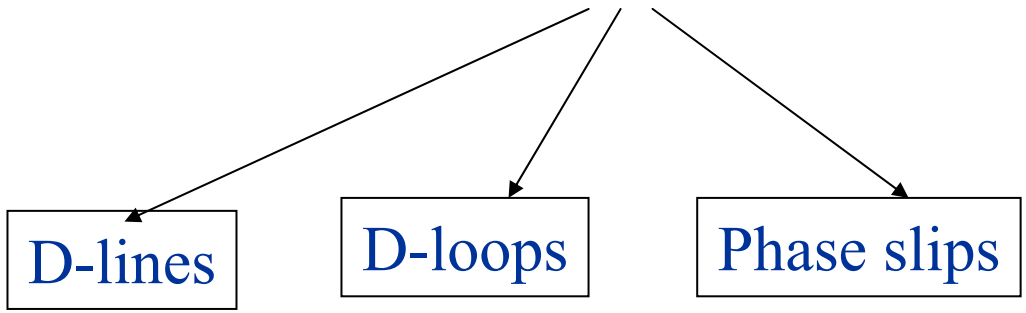
Macroscopically – edge dislocation line proliferating/expanding across the sample.



Adequate definition of ***plastic deformations/flows:***
distorted/sliding states of coherent media - crystals (superfluids) accompanied by local creation/annihilation of new periods.

Realization:

Electrons $\Rightarrow$ Amplitude solitons $\Rightarrow 2\pi$ phase solitons



Originated by:

- normal/collective current conversion
- surface strains
- impurities

History of dislocations in CDWs:
Dumas, Feinberg, Friedel, Maki, Gorkov, Gill, Brazovskii, Matveenko, Kirova, Thorne, Monceau, …

Our goal: theory of plastic flows of sliding superstructures

To describe:

- Current conversion: normal current ⇔ collective one
- Relaxation of injected carriers:
  normal electrons ⇔ crystal's periods
- Collective motion in constrained geometry
- Plastic contribution to nonlinear I-V

$\varphi = \omega t + kx^2/2$

$-\gamma\omega = \mathbf{C}E$

$-k^2 = (1-\mathbf{C})E$

Partition $\mathbf{C}$=?

$F_{frc}(\varphi)$

? which $\dot{\varphi}$

$$-\gamma\dot{\varphi} + \nabla^2\varphi = E$$

? which **E:**

$$\frac{\Phi}{L};\ \frac{V_{ps}}{L};\ \frac{J}{\sigma}$$

? which J

? which σ

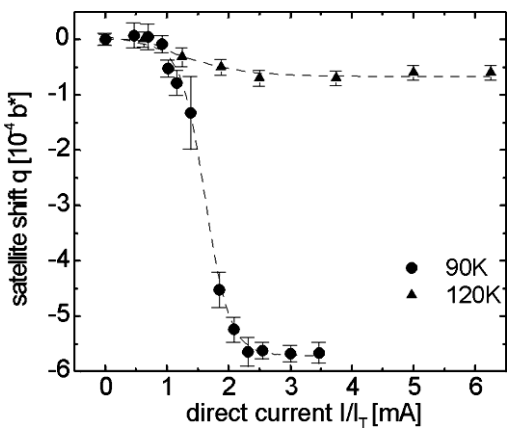
$\mathbf{f}(\nabla)\,\varphi$

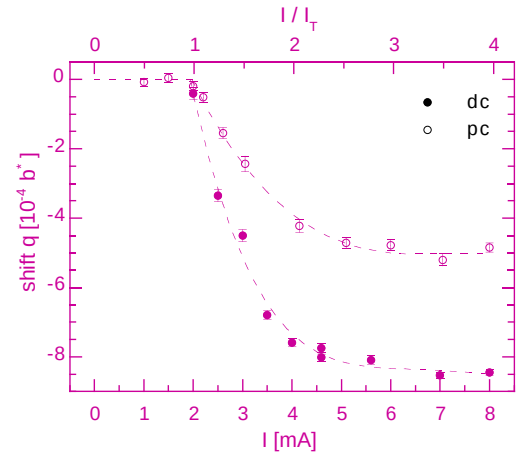
normal carriers

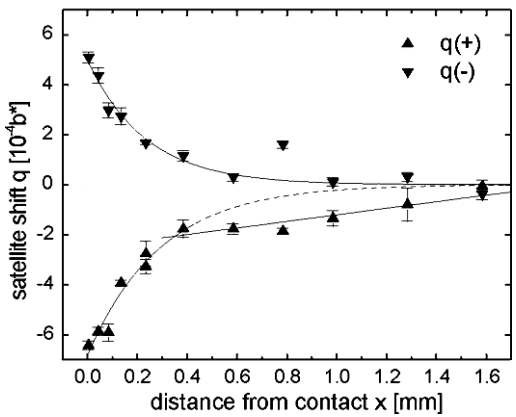
Coulomb

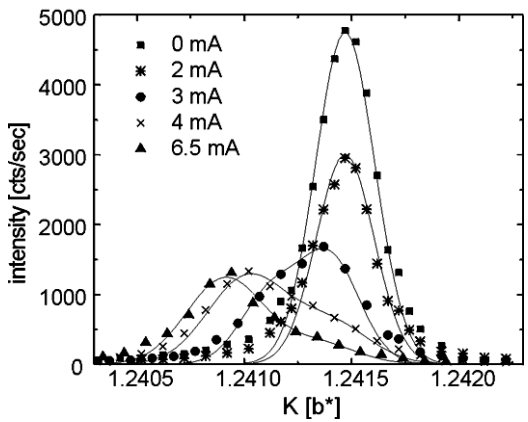
Current conversion

F. Nad' et al

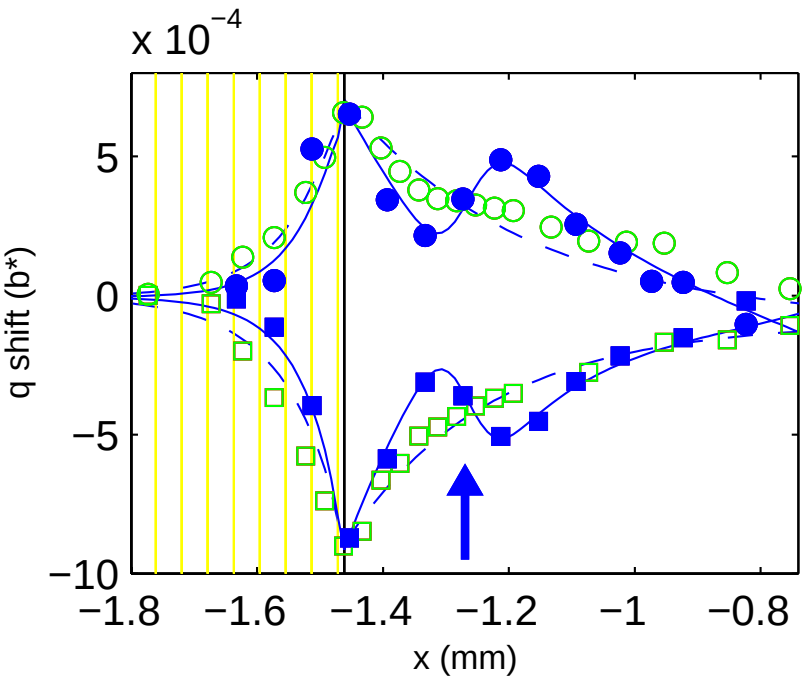


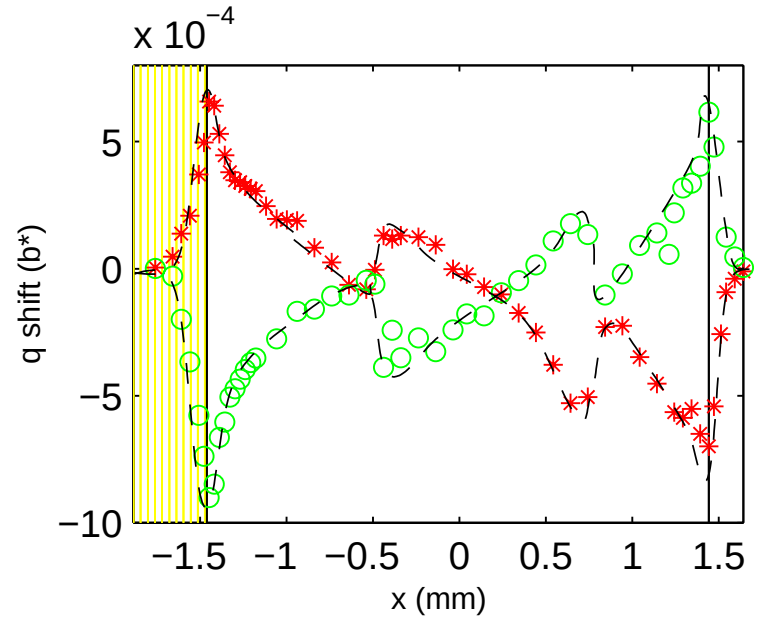


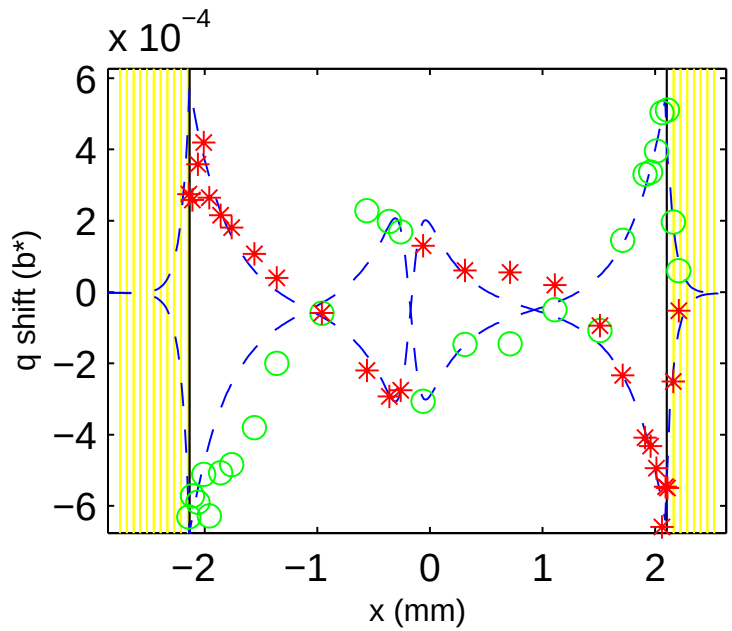




Plastic flows via space resolved diffraction







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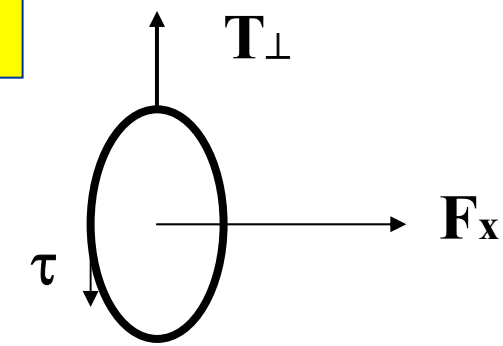
Two types of dislocation motion: Glide and Climb



Glide: Force ≠ energy gradient

$$\vec{F} \propto \int \left[\vec{T} \times d\vec{l}\right]$$

Supposed by analogy with magnetic forces:

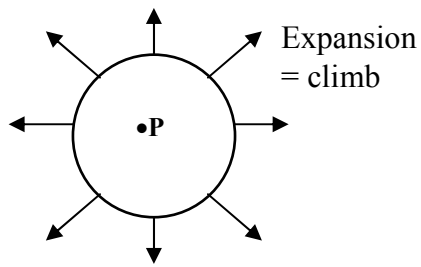
$$F_x \propto \oint \vec{T}_\perp \times d\vec{l} \Leftrightarrow -\frac{\partial}{\partial x} U = -\frac{\partial}{\partial x} \int \vec{T} d\vec{s}$$

Correct, because $\vec{\nabla}\vec{T} = F_{frc}(\dot{\varphi}) \neq 0$

wrong

Climb: non dynamic but kinetic process – dislocation growth.
$dn_d/dt \neq 0$, n_d – density of defects

$$F_\perp \propto \int T_x dl$$

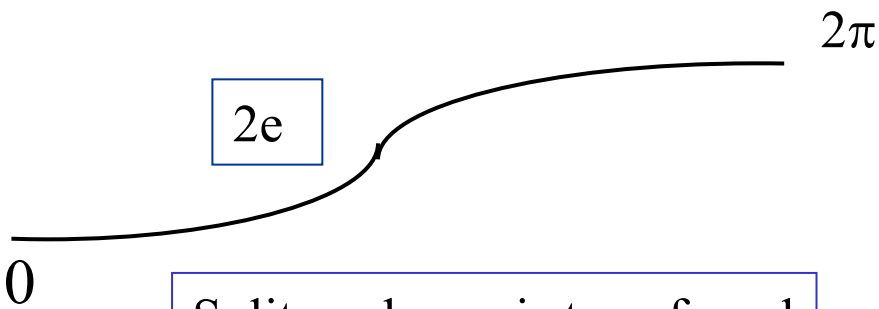


$F_\perp$ promotes climb – forbidden expansion of loop – mass/charge conservation.
Usual prescription: project out, then we loose conversion

Here : ***consider climb only as a grows by adhesion of normal carriers***

Glide : local versus integral currents.
Nucleolus dislocation loop ≡2π-solit

Does 2π ≡ 2e soliton glide under applied electric field E?
NO (YES for pinned DW.)



Local charge 2e, local current 2e v_x.
n=0 δφ=2π n≠0 δφ=0

Soliton charge is transferred to the collective mode

Compensating charge in long range tails

$$\varphi_{LR} \sim \frac{-xs}{\left(x^2+r_\perp^2\right)^{3/2}} \Rightarrow \int \frac{d^2 r_\perp}{s}\varphi_{LR} \equiv \bar{\varphi}_{LR}(x) = -\pi\,\mathrm{sgn}(x)$$

Glide: Force ≠ energy gradient

$$\vec{F} \propto \int \left[\vec{T}\times d\vec{l}\right]$$

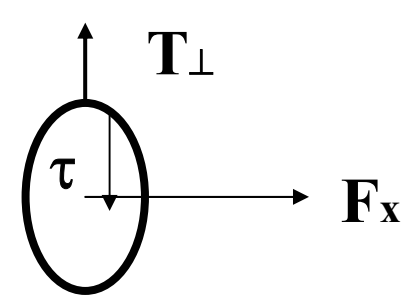
Long range tail charge -2e,
total charge =0
no integral current

Supposed by analogy with magnetic forces:

$$F_x \propto \oint \vec{T}_\perp \times d\vec{l} \Leftrightarrow -\frac{\partial}{\partial x}U = -\frac{\partial}{\partial x}\int \vec{T}d\vec{s}$$

Correct, by definition

Wrong, because
$\vec{\nabla}\vec{T} = F_{frc}(\dot{\varphi}) \neq 0$



We need: **a careful separation of various contributions to the current.**

Kinematics at presence of dislocation lines/loops (DL)
Geometric relations

Local deformations and velocities are not derivatives of the same phase

$$\frac{\partial\varphi}{\partial x}\to\varphi_x;\qquad \frac{\partial\varphi}{\partial y}\to\varphi_y;\qquad \frac{\partial\varphi}{\partial z}\to\varphi_z\qquad \frac{\partial\varphi}{\partial t}\to\varphi_t;$$

Four variables: $\boldsymbol{\varphi_x, \varphi_y, \varphi_z, \varphi_t}$ instead of one : $\boldsymbol{\varphi}$

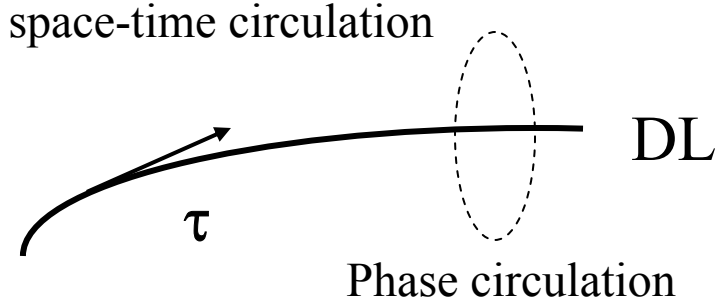
$(\varphi_x, \varphi_y, \varphi_z) = (\omega_x\ \omega_y\ \omega_z) = \boldsymbol{\omega}$ $\qquad$ $\boldsymbol{\omega}\neq\nabla\varphi \leftrightarrow \nabla\times\boldsymbol{\omega}\neq 0$

$$\vec{\tau} = \frac{1}{2\pi}\left[\nabla\times\vec{\omega}\right]$$ - density of dislocation lines, space circulation of φ

$$I = \frac{1}{2\pi}(\nabla\varphi_t - \frac{\partial\omega}{\partial t})$$ - flow of dislocation lines, space-time circulation

Compatibility relation

$$\vec{\nabla}\times\vec{I} = -\frac{\partial\vec{\tau}}{\partial t}$$



$$\vec{\nabla}\ \vec{\tau} = 0 \quad \Rightarrow \quad \vec{\tau} = -\frac{1}{2\pi}\left[\vec{\nabla}\times\vec{P}\right]$$

No terminations for dislocation lines.

P – density of discontinuities at arbitrary surfaces based on DL,

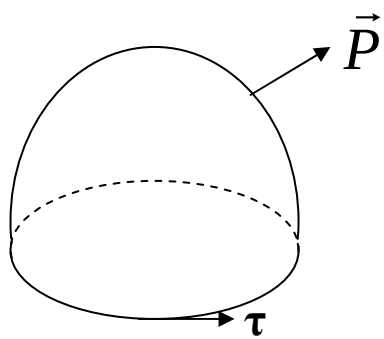
ω = -P up to the gradient of one valued function, ***call it the phase φ***

$$\vec{\omega} + \vec{P} = \vec{\nabla}\varphi$$

$$\vec{I} = \frac{\partial\vec{P}}{\partial t} + \frac{1}{2\pi}\left(\vec{\nabla}\varphi_t - \frac{\partial\vec{\omega}}{\partial t}\right)$$

τ,*I* - physical singularity on DL,

P, φ – non-physical singularities

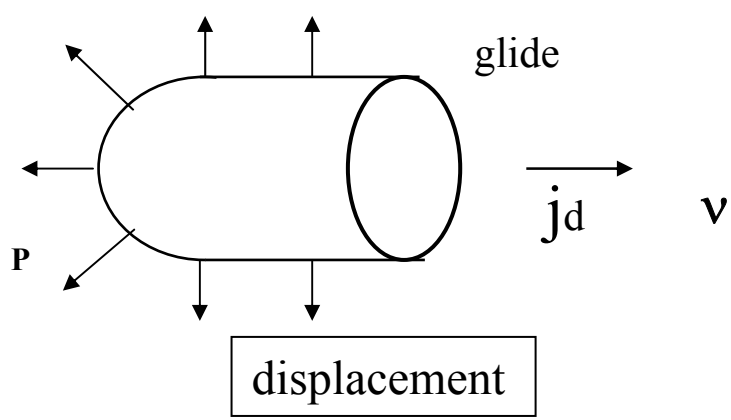


$$\vec{I} \propto \vec{v}_{DL} \times d\vec{l}$$

Fix the time dependent part of the gauge:

$$\varphi_t = \frac{\partial \varphi}{\partial t} \quad \Rightarrow \vec{\nabla}\varphi_t = \frac{\partial}{\partial t}\left(\vec{\omega} + \vec{P}\right) \quad \Rightarrow \quad \vec{I} = \frac{\partial \vec{P}}{\partial t}$$

φ_t, ω, I are singular on DL only. Now the same holds for $\vec{P}_t$ and $\vec{I}$.
Discontinuity surface $\vec{P}$ is arbitrary only at some initial t=0.
Afterwards $\vec{P}$ evolves only along the surface passed by DL,
that is following the trace of physical singularities.



$j_d \neq 0$, conservative motion , allowed only along ν

Averaging over DL distribution

From non-unique **P**, φ to unique $\mathbf{j}_d$, n_d

n_d – density of defects = DL area/volume

$\mathbf{j}_d=(j_d,0,0)$ – current of defects

$\langle P_x \rangle = 2\pi n_d$ – projected DL area/volume

$$-2\frac{dn_n}{dt} = \frac{dn_d}{dt} = \frac{\partial n_d}{\partial t} + \frac{\partial j_d}{\partial x}$$

$$\langle [\vec{\nu}\vec{\tau}] \rangle = -\vec{\nabla}_\perp n_d$$

$$\langle \vec{\tau} \rangle = -[\vec{\nu} \times \vec{\nabla}] n_d$$ - for plain loops

$$\vec{\nabla} \times \langle \vec{I} \rangle = -\frac{\partial}{\partial t}\langle \vec{\tau} \rangle = \left[\vec{\nabla} \times \vec{\nu}\frac{\partial n_d}{\partial t}\right] \Rightarrow \langle \vec{I} \rangle = \vec{\nu}\frac{\partial n_d}{\partial t} + \vec{\nabla} f$$

Identify unknown $f \equiv j_d$

$$\langle I_x \rangle = \left\langle \frac{\partial P_x}{\partial t} \right\rangle = 2\pi \frac{dn_d}{dt} = 2\pi\left(\frac{\partial n_d}{\partial t} + \frac{\partial j_d}{\partial x}\right)$$

$$\frac{1}{2\pi}\langle \vec{I} \rangle = \vec{\nu}\frac{\partial n_d}{\partial t} + \vec{\nabla} j_d$$

Climb: $$\left\langle \frac{\partial P_x}{\partial t} \right\rangle - \frac{\partial \langle P_x \rangle}{\partial t} = 2\pi \frac{\partial j_d}{\partial x} \neq 0$$

Glide: $$\left\langle \frac{\partial P_x}{\partial t} \right\rangle - \frac{\partial \langle P_x \rangle}{\partial t} = 0$$

Result: There is a uniquely defined function χ such that

$$\frac{\partial \chi}{\partial t} = \langle \varphi_t \rangle + 2\pi j_d \qquad \frac{\partial \chi}{\partial x} = \langle \varphi_x \rangle - 2\pi n_d \qquad \frac{\partial \chi}{\partial y} = \langle \varphi_y \rangle \qquad \frac{\partial \chi}{\partial z} = \langle \varphi_z \rangle$$

Finding χ is equivalent to find the first integral to four equations for φ_α , α=x,y,z,t.

A straightforward derivation

Forget the phases, follow stresses T_i, return to φ_α as self average values, average, find then separate Eqs. for $<\varphi_\alpha>$, try to find the first integral χ.

Procedure: Introduce **P** → noninvariant integration of φ_α to $\partial_\alpha\varphi$ →exclude unnecessary $\nabla_\perp\varphi$ →

Equation for physical variables: compression φ_x, field **E**

$$\frac{1}{\pi}\left(\hat{\Delta}-\gamma\frac{\partial}{\partial t}\right)\varphi_x+\frac{\partial E}{\partial x}-\frac{\partial^2 n_n}{\partial x^2}=\frac{\gamma}{\pi}\frac{\partial}{\partial t}\left(\vec{v}\vec{P}\right)+2\alpha\left(\left[\vec{\nabla}\times\vec{v}\right]\vec{\tau}\right)$$

R.H.S.$\Rightarrow$ $$2\gamma\frac{dn_d}{dt}-2\alpha\nabla_\perp n_d$$

Self averaging: L.H.S. – by definition
R.H.S. – by construction

Final equations:

Visco-elastic – plastic motion

$$\frac{1}{\pi}\left(\hat{\Delta}-\gamma\frac{\partial}{\partial t}\right)\chi=-\frac{\partial\Phi}{\partial x}-2\gamma j_d-\frac{\partial}{\partial x}\left(n_i+2n_d\right)$$

+

Poisson Eq.

$$r_0^2\Delta\Phi+n_n+2n_d+\frac{1}{\pi}\frac{\partial\chi}{\partial x}=0$$

From kinematics to dynamics.

Local material relations:

Velocity : $v=\varphi_t \leftarrow \partial\varphi/dt$

Strain : $\omega=\omega(T) \leftarrow \nabla\varphi$

Stress : $T=\delta W/\delta\omega$

Equilibrium:

$\nabla T=F_{frc}(v) \leftarrow m dv/dt+\gamma v$

DW specific relations:

Poisson equation: $\delta W/\delta\Phi=0$

Normal carriers:

Chemical potential : $\mu_n=\delta W/\delta n$

Current: $j_n=-\sigma_n\nabla\mu$

Conservation :

$$\frac{\partial n_n}{\partial t}+\nabla j_n=\frac{dn_n}{dt}$$

Source – drain = conversion

$$R(\mu_d-\mu_n)=\frac{dn_d}{dt}=-2\frac{dn_n}{dt}$$

$n_n=n_i+n_e$ – normal electrons

R- phase slip rate

Supplements: material relations and kinetics

Diffusion Eqs. for carriers: $\partial_t n - D\nabla^2 \mu = \frac{dn}{dt}$

$n_n = n_i + n_e$; $n_e = n_e(\Phi)$; $n_i = n_i(V)$; $n_d = n_d(U)$

$dn_d/dt = K(\mu_d - \mu_n)$

e, h : $\mu_n = \mu_{loc}^n(n) + V$; $V = e\Phi + \frac{v_F \hbar}{2}\varphi_x$

d : $\mu_d \neq \mu_{loc}^n(n) + U$ $\quad \frac{\partial \mu_d}{\partial x} = \frac{\partial \mu_{loc}^d}{\partial x} + \alpha \Delta_\perp \chi \neq \frac{\partial U}{\partial x}$

$$U = \Phi + \frac{\hbar v_F}{2}\varphi_x + \frac{\pi \hbar v_F}{2} n_i$$

DW stress contributions:

electric

elastic

inequilibrium

2U – energy per chain paid to distort the CDW elastically by one period

What would be without Coulomb interactions

$$\frac{1}{\pi}\left(\hat{\Delta}-\gamma\frac{\partial}{\partial t}\right)T_x=\frac{\partial F}{\partial x}+\hat{\Delta}_{\perp}\left(n_i+2n_d\right)+\gamma\frac{\partial j_n}{\partial x}+\dot{n}_{inj} \qquad T_x=U$$

Where does the stress come from?

- $\parallel$ gradient of external driving force F
- $\perp$ profile of both normal carriers and defects
- $\parallel$ gradient only of normal carriers
- charge injection

In terms of the invariant phase χ

$$\frac{1}{\pi}\left(\hat{\Delta}-\gamma\frac{\partial}{\partial t}\right)\chi=-2\gamma j_d+\frac{\partial}{\partial x}\left(2n_d+cn_i\right)+F$$

Driving force

D-loops

vacancies, addatoms

CDW reality: Coulomb forces, low T

$$-\gamma\frac{\partial}{\partial t}+\hat{\Delta}\Rightarrow\left[-\gamma\frac{\partial}{\partial t}-\hat{\Delta}_{\perp}^{2}+\frac{r_0^{-2}}{\Delta_{\perp}}\frac{\partial^2}{\partial x^2}\right]$$

nonlocal elasticity
S.B &S. Matveenko

$$\frac{1}{\pi}\left[r_0^2\Delta_{\perp}\left(\Delta_{\perp}-\gamma\frac{\partial}{\partial t}\right)-\underbrace{\frac{\partial^2}{\partial x^2}\Big]\chi=\frac{\partial}{\partial x}\left(n_n+2n_d\right)}_{\text{electroneutrality at } r_0=0}$$

Driving force: only || gradients of normal carriers and defects

1D regime: average crossection , $\langle\rangle_{r\perp}$

$\hbar v_F = 1$

Charge

$$\frac{1}{\pi}\frac{\partial \chi}{\partial x} + n_n + 2 n_d \equiv 0$$

Current

$$-\frac{1}{\pi}\frac{\partial \chi}{\partial t} + j_n + 2 j_d = J = cnst$$

Electric field actions in 1D

$$-\frac{\partial \Phi}{\partial x} = E = -\gamma \frac{\partial \chi}{\partial t} + 2\gamma\, j_d + \frac{\partial}{\partial x}\left(n_e + n_0\right)$$

Also a resolution of the dilemma:

$$\boldsymbol{E} = -\gamma \partial_t \varphi + k\varphi''$$

E *drives the DW motion:*

$\partial_t \chi + j_d \leftarrow$ the current of defects)

(together = total collective current)

E *withstands the || gradient of normal carriers concentration*

If $\partial_t \chi = 0$, then $V_{ps} = \Delta\Phi - EL = \hbar v_F n_e$
gives the access to extrinsic carriers at the contacts

Correlation of the DW stress and the normal chemical potential

$$-\frac{\partial}{\partial x}\left[T_x\sigma_c + \mu_n\sigma_n\right] = J_{tot}(t)$$

- DW is stressed only by normal carriers.
- Just the Kirchhof law –
  parallel circuits of collective current driven by
  – $\partial T_x/\partial x$ and $-\partial\mu_n/\partial x$ correspondingly

Conclusions

Modern experimental studies of CDW at constraint, meso & nano scales require for a transparent but complete description.
The presented scheme is a minimal version of the multi-fluid hydrodynamics of plastic flows.

Main theory ingradients:

Intrinsic carriers : from DOS N_F^i, closed by the gap: n_i, j_i, ρ_i, V_i.
Extrinsic carriers in semimetallic DWs ($NbSe_3$): their DOS fraction β_e is unaffected by the gap, n_e, j_e, V_e.

Collective variables : $\varphi_x = q$, $n_c = \varphi_x/\pi$; $j_c = -\varphi_t$; $\rho_c = 1 - \rho_i = \begin{cases} 1 & T = 0 \\ 0 & T = T_c \end{cases}$

Potentials : $V_e = \Phi$, $V_i = \Phi + q/\pi N_F^i$ ← reciprocal from banding

$$U = \Phi + \frac{\varphi_x}{\pi N_F^i} + \frac{n_i}{N_F^i}$$

DW stress contributions: U; Φ – electric; $\frac{\varphi_x}{\pi N_F^i}$ – elastic; $\frac{n_i}{N_F^i}$ – nonequilibrium

2U – energy per chain paid to distort the CDW elastically by one period

Viscosity force $\gamma\varphi_t$ and its generalization for the case of pinning

1D:

$$\gamma \frac{\partial \varphi}{\partial t} \to \begin{cases} F_{pin} & |F| < E_t \\ F_{frc}(j_c) & |F| > E_t \end{cases}$$

Local energy functional

$$W\{\varphi,\Phi,n\}=\frac{K_{\|}}{2}\left[\varphi_x^2+\alpha_y\varphi_y^2+\alpha_z\varphi_z^2\right]+\frac{e}{\pi}\varphi_x\Phi-\frac{s}{8\pi}(\nabla\Phi)^2+\frac{s}{4\pi}\left(\vec{E}\vec{D}\right)+en_e\Phi+\left(e\Phi+\frac{C}{2}\hbar v_F\varphi_x\right)n_i+W_n(n_i,n_e)$$

$$\varphi_i=\frac{\partial\varphi}{\partial x_i};\quad \frac{\varphi_x}{\pi}=\rho \text{ - charge density}$$

$\Delta\varphi=2\pi$ = CDW period = 2 electrons

CDW = Acos(Qx+φ), φ'=q=δQ

Φ - electric field potential,
$W_n(n_i,n_e)$ - free energy of normal carriers,
e - free electron charge, s - area per one chain,
E and D - electric field and induction,
n_i, n_e - concentrations of intrinsic and extrinsic free carriers,
C=1 and $K_{\|} = \hbar v_F/2$ - links to chiral invariant and chiral anomaly

What do we get when we measure :

$$E = F_{frc}(j_c) - \beta_e \frac{\partial q}{\partial x}\frac{g}{\pi N_F^i} = \beta_i F_{frc} + \beta_e \frac{j_{tot} - j_c}{\sigma_n}$$

$$g = g(T) = \frac{\rho_c}{\rho_c} \rightarrow \begin{cases} 0 & T \rightarrow T_c \\ \infty & T \rightarrow 0 \end{cases}$$

compressibility

Only in semiconducting DWs (β_e=0) electric field E gives access to friction.
At $\beta_e \neq 0$ strain contributes ($NbSe_3$, some DWs)

$$\frac{\partial}{\partial x} q \frac{g}{\pi N_F^i} = F_{frc}(j_c) - \frac{j_{tot} - j_c}{\sigma_n} \qquad \textbf{A}$$

e.g. to get $j_c(x,t)$ from measured $q(x,t)$

$$\frac{\partial q}{\partial t} + \frac{\partial j_c}{\partial x} = 2R(q, j_c) - v_{inj} \qquad \textbf{B}$$

Access to the phase slip rate R as a function of j_c and $q \sim \eta$

$$\frac{gq}{\pi N_F^i} = \mu_n - U \equiv \eta$$

A & **B** – full system of Eqs. to describe a space –time evolution