Charged density wave structure near contacts

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The structure of a distorted charge-density wave (CDW) near a lateral metallic surface is considered. It is shown that charge penetration and electric-field screening are realized through a nonuniform distribution of solitons or dislocations. Self-consistent equations of elasticity theory for CDW with topological defects are solved with allowance for accompanying Coulomb fields. For relatively high temperatures distributions of soliton-gas density and field over the sample depth are found and the contact capacitance is calculated. For low temperatures and densities, the fields and induced charges of a solitary dislocation under the metallic surface are studied at length. A periodic dislocation structure arises for certain critical difference of the CDW and metal potentials. For small charges near the threshold the dislocations are far apart and, unexpectedly, at a large depth. Thus, the contact region is a natural generator and accumulator of CDW topological defects which can serve as nuclei of phase-slippage centers when longitudinal current flows through the sample.

1. INTRODUCTION

Solitons and dislocations determine stable excited or distorted states of a CDW crystal and/or the dynamics of normal current conversion into CDW current (see citations in Refs. 1–4). We will show that these topological deformations inevitably arise in an electric field near the characteristic lateral contact of a CDW crystal with a metal. Thus, the region under the contact is a natural accumulator of topological defects which become activated by CDW slippage in fields higher than the critical one. The results could account for some experimental data on dislocations[5,6] and new experiments on potential distributions assymetry.[1)]

Let a CDW crystal occupy the half-space $y > 0$, and let the contact with a metallic electrode be in the xz plane (the x axis coincides with the chain direction). Let the value of electric potential in the crystal depth be zero (here and in what follows Φ is the potential energy of a particle with a one-electron charge $e > 0$):

$$\Phi_{\times}(x, y=\infty)\equiv 0,\ \Phi(x, 0)\equiv\Phi_0>0. \tag{1}$$

The metal potential with respect to the CDW, Φ_0, is determined, for example, by the difference in the work functions but it can also be controlled in the field effect regime (a dielectric interlayer). In what follows we consider low temperatures $T \ll \Delta$, where 2Δ is the gap width in the electron spectrum, when the electron density is low.

The reason why topological defects are needed to screen an electric field, i.e., to satisfy both conditions (1), is the following. To create a CDW charge density

$$\rho=\frac{1}{\pi s}\frac{\partial\varphi}{\partial x},\qquad s=a_y a_z$$

(s is the area per chain, and a_y and a_z are the distances between the chains) that is inhomogeneous in y, the CDW wave vector should change by $\delta q = (\partial^2\varphi/\partial x\partial y)a_z$ between the neighboring, with respect to the y axis, chain layers. This could lead to a loss in the total energy of three-dimensional ordering, of order T_c^2/v per chain unit length ($\hbar = k_B = 1$, T_c is the temperature of $3d$-ordering, and v is the Fermi velocity) for infinitesimal charge redistribution. This situation resembles the distributed commensurability effect. It is evident that the energy loss per charge $2e$ is finite, if incommensurability of neighboring chains is concentrated in the form of 2π-solitons (see Refs. 1 and 2) with charge $2e$, length $l\sim v/T_c$, and energy $E_s \sim T_c$. At low temperatures, soliton aggregation into filaments along the z axis and their correlation along the y axis is advantageous. These cases are naturally classified in terms of dislocations.[3,4]

One soliton or a limited soliton complex corresponds to a dislocation loop enclosing one or several chains. A soliton line corresponds to a dislocation loop extended along the z axis. Total aggregation from the surface to some depth Y corresponds to a single dislocation line passing parallel to the z axis through the point $y = Y$, for some x. According to the results of Refs. 1–4, the threshold value of Φ_0 for the beginning of charge penetration, and consequently screening, is equal, for the cases listed above, to E_s, $\widetilde{E}_s$ and μ_0 respectively, where the energies $E_s \sim (\alpha/s)^{1/2}$ and $\widetilde{E}_s \sim v(\tilde{\alpha}/s)^{1/2}$ are determined by the largest (α) and the smallest ($\tilde{\alpha}$) structural-anisotropy parameters.[1–4] The value $\mu_0 \sim \alpha_y^{1/2}\omega_p$, where ω_p is the plasma frequency, can be both larger and smaller than E_s.[3,4]

2. CONDITIONS OF CDW EQUILIBRIUM NEAR A LATERAL CONTACT

The continuous distribution of dislocations (see Refs. 7 and 8) or solitons in the CDW is given by the vectors $\boldsymbol{\rho}$ or $\mathbf{P}$, which are connected by the relation $\boldsymbol{\rho} = [\nabla\mathbf{P}]$. For one dislocation we have

$$\boldsymbol{\rho}dV=-2\pi\delta(\boldsymbol{\xi})d\mathbf{l},\quad \mathbf{P}dV=-2d\mathbf{s},$$
$$d\mathbf{l}=\boldsymbol{\tau}dl,\quad |\boldsymbol{\tau}|=1,\quad \boldsymbol{\xi}\boldsymbol{\tau}=0, \tag{2}$$

where $d\mathbf{l}$ is the dislocation line length element, and $d\mathbf{s}$ is the element of the phase-discontinuity surface φ. For a $\pm 2\pi$-soliton at the point $\mathbf{r} = 0$

$$\mathbf{P}=(P,\ 0,\ 0),\quad \mathbf{P}=\mp 2\pi s\mathbf{n}\delta(\mathbf{r}), \tag{3}$$

where $\mathbf{n}$ is the x-axis direction. Hereafter we define the phase as a single-valued and, generally speaking, discontinuous function of the CDW, which corresponds to the field φ in Refs. 3 and 4. It is connected with the locally defined contin-

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uous phase gradient ω by the relation

$$\nabla\varphi=\omega+\mathbf{P}. \tag{4}$$

The fields $\omega\mathbf{n}/\pi$ and $-\dot{\varphi}/\pi$ determine the CDW charge density and total current. General equilibrium conditions,[3,4] in terms of φ and $\mathbf{P}$, take the form

$$(\mathbf{n}\nabla)[\hat{\nabla}(\nabla\varphi-\mathbf{P})+(2/v)(\mathbf{n}\nabla)\Phi]=0. \tag{5}$$

$$(2/v\varkappa^2)\Delta\Phi+n(\nabla\varphi-P)=0, \tag{6}$$

where

$$\hat{\nabla}=\left(\frac{\partial}{\partial x},\alpha_y\frac{\partial}{\partial y},\alpha_z\frac{\partial}{\partial z}\right),\quad \varkappa^2=\frac{8e^2}{vs},\qquad v\varkappa=\omega_p,$$

$\varkappa$, ω_p and v are the inverse Debye radius, plasma frequency and Fermi velocity of the metal respectively, and α_y and α_z are parameters of the CDW elastic anisotropy. Note that for solitons we always have $\mathbf{P}$ and $\mathbf{n}P$, and for the transverse plane dislocations we can always choose the vector $\mathbf{P}$ in the same way. Recall also[1,2] that the field

$$2V=2\Phi+v\omega_x=2\pi v\sigma\mathbf{n},\quad \omega_x=\partial\varphi/\partial x-P, \tag{7}$$

where σ is the CDW stress vector, is the potential energy of a 2π-soliton and also the transverse force acting upon a unit length element in the direction perpendicular to the dislocation line.

3. HIGH TEMPERATURE: SOLITON GAS

Consider now the case of high soliton or dislocation density, when P can be considered a continuous function depending only on y. Equations (5) and (6) take the form

$$\frac{\partial}{\partial x}\hat{\Delta}\varphi=0,\quad \varphi=\varphi(x,y), \tag{8}$$

$$\frac{2}{\varkappa^2 v}\frac{\partial^2\Phi}{\partial y^2}+\frac{\partial\varphi}{\partial x}-P=0,\quad P=P(y),\quad \Phi=\Phi(y). \tag{9}$$

where

$$\hat{\Delta}=\nabla\hat{\nabla}=\frac{\partial^2}{\partial x^2}+\alpha_y\frac{\partial^2}{\partial y^2}+\alpha_z\frac{\partial^2}{\partial z^2}.$$

To close this system it is necessary to add the equation of equilibrium with respect to the P-distribution. We will consider the range of fairly high temperatures T and/or strong Coulomb interaction (see Refs. 3 and 4), when $\mu_0>E_s$. In these cases the number of dislocations or multielectron dislocation loops is small, and the value of P is given by the soliton Boltzmann distribution

$$P=2\pi(\rho_- -\rho_+),\quad \rho_\pm=d^{-1}\exp\{-\beta[E_s\pm(V-\mu)]\}. \tag{10}$$

Here $\rho_\pm$ and $\pm\mu$ are the density and chemical potentials of $\pm 2\pi$-solitons respectively, and $\beta=1/T$. The length d depends on the character of configurational averaging. For quantum solitons $d\sim(MT)^{-1/2}$, where $M\sim T_c/u^2$ is the soliton mass and u the CDW phase velocity. For pinned solitons d is the distance between defects along a chain. A finite displacement $\mu\neq0$ in the absence of conduction electrons is caused by microscopic charge asymmetry. The latter stems from dispersion of $2k_F$- phonons.[9] As a result,

$$\mu\propto\Delta^3 c/\overline{\omega}g^2, \tag{11}$$

where $|\mu|<E_s$, c is the sound velocity, $\overline{\omega}$ is the $2k_F$-phonon frequency, and g is the electron–phonon interaction constant.

The inequality in (11) ensures ground-state stability. In the bulk we have from (1) and (7)–(9)

$$y\to\infty:\quad \Phi\to0,\ P\to P_\infty,\ \partial\varphi/\partial x\to P_\infty,\ \omega_x\to0. \tag{12}$$

The last condition means electroneutrality. Equation (10) yields

$$P_\infty=-A\,\mathrm{sh}\,\beta\mu,\ A=(4\pi/d)\exp(-\beta E_s). \tag{13}$$

The only nonsingular solution of Eq. (8), which satisfies (11), has the form

$$\varphi=P_\infty x. \tag{14}$$

It means that absolute CDW displacements are independent of the depth y despite the presence of solitons or dislocations. Equations (9), (10) and (14) yield a system of equations in $\Phi(y)$ and $P(y)$:

$$\frac{2}{\varkappa^2 v}\frac{\partial^2\Phi}{\partial y^2}-P+P_\infty=0, \tag{15}$$

$$2\Phi=\mu-vP_\infty+vP+T\,\mathrm{arcsh}(P/A). \tag{16}$$

Equations (7) and (15) have, in the general case, a first integral corresponding to conservation of the total energy density:

$$\frac{2}{\varkappa^2 v}\left(\frac{\partial\Phi}{\partial y}\right)^2+\Omega(\mu-2\Phi)+\frac{v}{2}P^2=\mathrm{const}, \tag{17}$$

$$\Omega\approx\Omega_s(\mu-2\Phi-E_s)-\Omega_s(-\mu+2\Phi-E_s), \tag{18}$$

$$\Omega_s(\zeta)\propto(T/d)\exp(\zeta/T). \tag{19}$$

Equation (17), where Ω is the thermodynamic potential of the soliton system, is exact in the adopted local-equilibrium scheme. The expression (18), where Ω_s is the partial potential of solitons having the same sign, corresponds to the gas approximation. The formula (19), which is equivalent to Eq. (16), corresponds to Boltzmann statistics. Next we consider, for definiteness, the case of $+2\pi$-solitons, therefore $P<0$.

Equations (16)–(19) are solved by quadratures. As a result, we find the following dependences.

Near the contact we have for $|P|\gg T/v,A$

$$P\approx2v^{-1}\Phi\approx2v^{-1}\Phi_0e^{-\varkappa y}. \tag{20}$$

Thus, the initial potential $\Phi_0\sim\Delta$ induces a high density of the order of the limit $P\sim\varkappa$, which rapidly decreases over microscopic distances to the limiting thermal density $P_T\sim T/v$. In the intermediate range $A\ll|P|\ll T/v$ we have

$$P\sim-T/v(\varkappa y)^2,\ \Phi\sim\ln y. \tag{21}$$

For still smaller $|P|\ll A$ the power law is replaced by a weak exponential dependence

$$P\sim-Ae^{-\delta y},\quad \delta\approx\varkappa(vA/2T)^{1/2}\ll\varkappa. \tag{22}$$

At last, for equilibrium density we have the regime of linear Debye screening in a weakly perturbed soliton gas:

$$P-P_\infty\propto e^{-\lambda y},\ \lambda=\varkappa(P/T)^{1/2}. \tag{23}$$

Here λ coincides with the parameter of screening by residual carriers in Refs. 1–4.

The obtained dependences allow to find, for example, the capacitance C or incremental capacitance $\tilde{C}$ per unit contact area S:

$$C=\frac{1}{\pi}[\Phi^{-1}\Phi']_{y=0}, \quad \tilde{C}=\frac{1}{\pi}\left[\frac{\partial\Phi'}{\partial\Phi}\right]_{y=0}. \tag{24}$$

Depending on the values $P_0=P(0)$ or $\Phi_0=\Phi(0)$, we have:

(a) for high density $|P_0|\approx 2|\Phi_0|/v\gg T$

$$C\approx\tilde{C}\approx\varkappa^{-1},$$

i.e., the capacitance is given by a microscopic layer of order $\varkappa^{-1}$, where the main charge is concentrated, and

(b) for low density $|P_\infty|\ll|P|\ll T$

$$C\propto\varkappa^{-1}\frac{(|P_0|v/T)^{1/2}}{\ln(P_0/P_\infty)}, \quad \tilde{C}\propto\varkappa^{-1}\left(\frac{|P_0|}{T}\right)^{1/2}, \tag{25}$$

where $P_0\approx P_\infty\exp(-\Phi_0/T)$.

Consider now the regime of stationary transverse current j flowing in the sample. It is natural to assume that the coefficient of transverse soliton diffusion $D=bT$ and the soliton mobility b are small so that CDW deformations can be regarded as static. As before, Eq. (15) holds, but instead of (16) we must use the generalizing diffusion equation

$$j=-D\frac{\partial\rho}{\partial y}-b\rho\frac{\partial V}{\partial y}, \quad P=-2\pi\rho. \tag{26}$$

Conditions (1) are replaced by

$$E=-\frac{\partial\Phi}{\partial y}\to E_\infty=\frac{j}{b\rho_\infty}, \quad y\to\infty. \tag{27}$$

For the sake of simplicity, we assume again that only one type of carrier dominates. As a result, we find an equation for E:

$$TE''+(E''\varkappa^{-2}-E)(2E'+T\lambda^2)+2T\lambda^2E_\infty=0, \qquad \rho/\rho_\infty=E'/T\lambda^2. \tag{28}$$

For small $E_\infty\propto j$ we find the regimes (20) and (21). However for large y, instead of (23), we get

$$E-E_\infty\propto e^{-ky}, \quad k=[(\beta E_\infty)^2+\lambda^2]^{1/2}-\beta E_\infty. \tag{29}$$

The effect of E_∞ is important for

$$E_\infty\gg\lambda T, \quad k\approx\lambda^2/2\beta E_\infty, \tag{30}$$

i.e., when the potential variation in the bulk over the screening length λ is large in comparison with temperature. In this case the field diffusion penetration length k^{-1} is large compared with the thermodynamic quantity λ.

4. LOW DENSITY AND TEMPERATURE: SINGLE DISLOCATIONS

As shown in Refs. 3 and 4, under the condition of sufficiently weak Coulomb interaction or under screening by residual carriers solitons begin to aggregate into macroscopic dislocations. In this section we study the properties of single dislocations near the lateral surface $y=0$. The lateral surface leads to a substantial change in the CDW deformation and electric potential around a dislocation, as well as to a change in dislocation energy. The results are different for the boundary with a dielectric and for the boundary with a metal.

To generalize the equilibrium conditions (5) and (6) for an infinite CDW crystal, we write the Hamiltonian in the form:[2]

$$H=\int_{y>0} d^3r\frac{v}{2\pi s}\left[\frac{(\hat{\nabla}\varphi-\mathbf{P})^2}{2}+\frac{2}{v}\left(\frac{\partial\varphi}{\partial x}-P_x\right)\right.$$
$$\left.+\frac{2}{\varkappa^2v^2}(\lambda^2\Phi-(\nabla\Phi)^2)+\rho(x)\delta(y)\right], \tag{31}$$

where $\mathbf{P}$ is the density of soliton or dislocation dipole moment, λ^{-1} is the residual carrier screening length, and $\rho(x)\delta(y)$ is the surface charge density arising at the boundary with a metal.

Consider, first, one dislocation loop lying in the plane $x=0$ and stretched along the z axis ($L_z\to\infty$). In this case the dislocation loop degenerates into two dislocation lines given by the equations $x=0, y=Y_1$ and $x=0, y=Y_2$, and the solutions for the fields φ and Φ are z independent of z. The case $Y_1=0$ corresponds to one dislocation split from the surface $y=0$. In this case

$$\mathbf{P}=-2\pi\theta(y-Y_1)\theta(Y_2-y)\delta(x)\mathbf{n}.$$

Varying the functional (31) with respect to the fields φ and Φ, we get the equilibrium conditions

$$\hat{\Delta}\varphi+\frac{2}{v}\frac{\partial\Phi}{\partial x}=\frac{\partial P_x}{\partial x}, \quad \hat{\Delta}=\frac{\partial^2}{\partial x^2}+\alpha_y\frac{\partial^2}{\partial y^2}, \tag{32}$$

$$\frac{2}{\varkappa^2v}(\Delta-\lambda^2)\Phi+\frac{\partial\varphi}{\partial x}=P_x-\rho(x)\delta(y), \tag{33}$$

from which the equations for the fields φ and Φ are easily obtained:

$$\hat{K}\Phi=-\pi\varkappa^2v\alpha\frac{\partial}{\partial y}[\delta(y-Y_1)-\delta(y-Y_2)]\delta(x)-\frac{\varkappa^2v}{2}\hat{\Delta}\rho(x)\delta(y), \tag{34}$$

$$\hat{K}\frac{\partial\varphi}{\partial y}=-2\pi(\varkappa^2+\lambda^2-\Delta)\frac{\partial}{\partial x}\delta(x)[\delta(y-Y_1)-\delta(y-Y_2)]$$
$$+\varkappa^2\frac{\partial}{\partial x}\rho(x)\frac{\partial}{\partial y}\delta(y), \tag{35}$$

where

$$\hat{K}=(-\lambda^2+\Delta)\hat{\Delta}-\varkappa^2\frac{\partial^2}{\partial x^2}.$$

For one dislocation line, without allowance for boundary effects, Eqs. (34) and (35) yield an exact (for $\alpha=1$, $\lambda=0$) solutions (see Refs. 3 and 4)

$$\Phi_0=\frac{\varkappa v}{2}\left(\operatorname{ch}\tilde{x}-\operatorname{sh}\tilde{x}\frac{\partial}{\partial x}\right)\int_0^{\tilde{y}}K_0((\tilde{x}^2+z^2)^{1/2})\,dz, \tag{36}$$

$$\frac{\partial\varphi_0}{\partial y}=-\frac{\varkappa^2-\Delta}{\varkappa}K_0((\tilde{x}^2+\tilde{y}^2)^{1/2})\operatorname{sh}\tilde{x}, \tag{37}$$

where $\tilde{x}=\varkappa x/2$, $\tilde{y}=\varkappa y/2$, and K_0 is a modified Bessel function, and the approximate solutions

$$\Phi_0=\frac{\pi\varkappa v\alpha^{1/2}}{4}\operatorname{erf}\left(\left[\frac{\varkappa y^2}{4\alpha^{1/2}|x|}\right]^{1/2}\right)\operatorname{sign}y, \tag{38}$$

$$\frac{\partial\varphi}{\partial y}=-\left(\frac{\varkappa\pi}{4\alpha^{1/2}|x|}\right)^{1/2}\exp\left(-\frac{\varkappa y^2}{4\alpha^{1/2}|x|}\right)\operatorname{sign}x, \tag{39}$$

are valid for $\lambda=0$, $y\gg\alpha^{1/2}x$ [erf(...) is the probability integral], and also solutions for $\lambda\neq 0$:

$$\Phi_0=\frac{\varkappa v\alpha^{1/2}}{2}y\frac{1}{y^2+\alpha^* x^2}. \qquad (40)$$

$$\frac{\partial\varphi_0}{\partial y}=-\frac{\alpha^{1/2}\lambda}{\varkappa}x\frac{1}{y^2+\alpha^* x^2} \qquad (41)$$

in the region $x\gg\varkappa/(\alpha^{1/2}\lambda^2)$, $y\gg\lambda^{-1}$, where $\alpha^*=\alpha\lambda^2/\varkappa^2$ is the effective anisotropy constant.

Now we take into account the boundary effect. Varying the functional (4), we obtain the boundary conditions

$$\left.\frac{\partial\varphi}{\partial y}\right|_{y=0}=0,\qquad \left.\frac{\partial\Phi}{\partial y}\right|_{y=0}=0 \qquad (42)$$

for the vacuum interface and the conditions

$$\left.\frac{\partial\varphi}{\partial y}\right|_{y=0}=0,\qquad \Phi|_{y=0}=0\rightarrow\frac{2}{\varkappa^2 v}\left.\frac{\partial\Phi}{\partial y}\right|_{y=0}+\rho(x)=0 \qquad (43)$$

for the metal interface.

Consider, first, the case of vacuum interface ($\rho(x)=0$). Dislocation lines at points $y=Y_1$ and $y=Y_2$ have opposite directions of the tangent vector $\boldsymbol{\tau}=\pm\mathbf{z}$ ($\mathbf{z}$ is the unit vector along the z axis), therefore it is convenient to attribute to them topological charges ± 1. The fields φ and Φ around these lines differ in sign. Equations (36)–(41) show that the boundary conditions (42) are identically satisfied if imaginary dislocation lines with opposite topological charges ± 1 are placed above the CDW crystal at symmetric points $x=0, y=-Y_1$ and $x=0, y=-Y_2$. Then the solution for Φ has the form and the function φ is given by a similar expression

$$\Phi=\Phi_0(y-Y_1)-\Phi_0(y+Y_1)-\Phi_0(y-Y_2)+\Phi_0(y+Y_2) \qquad (44)$$

Let us now find the solution of Eqs. (34) and (35) for the boundary with a metal. It is easy to see that the boundary condition $\Phi=0$ is not satisfied for the solutions (44), if $y=0$, therefore it is necessary to allow for external electric charge localized at the interface.

Without screening ($\lambda=0$) Eqs. (34) and (35) yield

$$\Phi=\Phi_0(x,y-Y)-\Phi_0(x,y+Y)-(\varkappa^2 v/2)\mathscr{E}_2*\rho(x)\delta(y), \qquad (45)$$

where

$$\mathscr{E}_2=\frac{1}{2\pi}K_0(\tilde{x}^2+\tilde{y}^2)^{1/2})\operatorname{ch}\tilde{x}$$

is the solution of the equation

$$\hat{K}\mathscr{E}_2=\Delta\delta(x,y).$$

Similarly, for φ we have

$$\frac{\partial\varphi}{\partial y}=\frac{\partial\varphi_0(x,y-Y)}{\partial y}-\frac{\partial\varphi_0(x,y+Y)}{\partial y}+\mathscr{E}_1*\varkappa^2\rho(x)\frac{\partial}{\partial y}\delta(y), \qquad (46)$$

where

$$\mathscr{E}_1=-\frac{1}{2\pi\varkappa}K_0((\tilde{x}^2+\tilde{y}^2)^{1/2})\operatorname{sh}\tilde{x}$$

is the solution of the equation

$$\hat{K}\mathscr{E}_1=\partial\delta(x,y)/\partial x$$

and

$$f*g=f(x-x')g(x')dx.$$

The Eqs. (45) and (46) are valid for one dislocation, $Y_1=0$ $Y_2=Y$ and are generalized to the case $Y_1\neq 0$ by the substitution $f(Y)\rightarrow f(Y_1)-f(Y_2)$.

It follows from (46) that an arbitrary external surface charge $\rho(x)$ does not alter the value of $\partial\varphi/\partial y$ for $y=0$, i.e., the first of the boundary conditions (43) is identically satisfied for any smooth function $\rho(x)$. Therefore the charge distribution density is unambiguously given by the second boundary condition (43) $\Phi|_{y=0}=0$. Substituting the approximate solutions (38) into (45) and using the boundary condition (43), we find

$$\rho(x)=-\frac{16\alpha^{1/2}}{\varkappa Y}\int_0^\infty e^{-t}\sin t\cos\left(\frac{2x\alpha^{1/2}}{Y^2\varkappa}t^2\right)dt. \qquad (47)$$

The asymptotes of Eq. (47) for small and large x have the form

$$\rho(x)\propto\begin{cases}-8/\varkappa Y, & 2x\alpha^{1/2}/Y^2\varkappa\ll 1,\\ -(\pi\varkappa)^{1/2}Y^2/|x|^{3/2}\alpha, & 2x\alpha^{1/2}/Y^2\varkappa\gg 1.\end{cases}$$

The total electric charge Q induced on the metallic surface cancels exactly the total electric charge of the solitons in the dislocation, and is distributed in the region $x\approx\varkappa Y^2/\alpha^{1/2}$:

$$Q=\frac{L_z}{s}\int_{-\infty}^{+\infty}\rho(x)dx=-2N, \qquad (48)$$

where N is the number of chains between the dislocation line and the surface, which corresponds to the number of 2π-solitons forming the dislocation.

In the same approximation Eq. (45) yields for the function Φ:

$$\Phi=\Phi_0(x,y-Y)-\Phi_0(x,y+Y)+\delta\Phi, \qquad (49)$$

where $\delta\Phi$ is the field of the charge $\rho(x)$:

$$\delta\Phi=-2\varkappa v\alpha^{1/2}\int_0^\infty\frac{dt}{t}\exp\left[-\left(1+\frac{Y}{y}\right)t\right]\sin\left(\frac{Y}{y}t\right)(\cos t-\sin t)\times\cos\left(\frac{2x\alpha^{1/2}}{\varkappa y^2}t^2\right). \qquad (50)$$

For $x=0$, Eqs. (49) and (50) yield an exact expression for Φ ($y>0$):

$$\Phi=\frac{\pi\varkappa v\alpha^{1/2}}{2}\theta(Y-y)-\varkappa v\alpha^{1/2}\operatorname{arctg}\left(\frac{Y}{y}\right)+\frac{\alpha^{1/2}\varkappa v}{2}\ln\frac{(y+Y)^2}{y^2+Y^2},$$

from which it follows that $\Phi(y)\rightarrow 0$ as $y\rightarrow 0$ and $\Phi\propto-\varkappa vY^2/y^2$ as $y\rightarrow+\infty$. The asymptotes (49) in different regions have the form

$$\Phi\approx\frac{(2\pi)^{1/2}\varkappa v\alpha^{1/2}}{4}Y^2y\left(\frac{\varkappa}{x}\right)^{3/2}$$

for

$$\frac{\varkappa y^2}{4\alpha^{1/2}|x|},\quad\frac{\varkappa Y^2}{4\alpha^{1/2}|x|}\ll 1 \qquad (51)$$

and

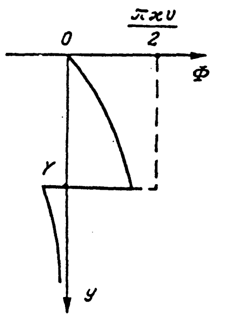

FIG. 1. Potential as a function of y in the plane $x = 0$ for a dislocation located at the point $(0,Y)$. At $x \neq 0$ the extrema are smoothed out and decrease.

$$\Phi \approx -\frac{\alpha^{1/4}(\pi\varkappa)^{1/2}v|x|^{1/2}}{y}\exp\left(-\frac{y^2}{4\alpha^{1/2}|x|}\right)\left[\frac{Y}{y}\operatorname{ch}\left(\frac{\varkappa yY}{2\alpha^{1/2}|x|}\right)\right.$$
$$\left.+\operatorname{sh}\left(\frac{\varkappa yY}{2\alpha^{1/2}|x|}\right)\right]-\varkappa v\alpha^{1/2}\operatorname{arctg}\left(\frac{Y}{y}\right)+\frac{\varkappa v}{2}\ln\frac{(y+Y)^2}{y^2+Y^2} \tag{52}$$

for

$$\frac{\varkappa Y^2}{4\alpha^{1/2}|x|}, \quad \frac{\varkappa y^2}{4\alpha^{1/2}|x|} \gg 1.$$

The function $\Phi(0,y)$ has for $y \lesssim Y$ a positive maximum approximately equal to $\alpha^{1/2}\varkappa v$ and and for $y \gtrsim Y$ a negative maximum approximately equal to $-0.5\,\alpha^{1/2}\varkappa v$. Thus, there is a region of attraction of electrons and solitons, which makes possible dislocation of growth into the interior. The function $\Phi(0,y)$ is plotted in Fig. 1.

In a similar way, we find for the function φ:

$$\varphi=\varphi_0(y-Y)-\varphi_0(y+Y)+\delta\varphi, \tag{53}$$

where

$$\delta\varphi=8\int_0^\infty \frac{dt}{t}\exp\left[-\left(1+\frac{Y}{y}\right)t\right]\sin\left(\frac{Y}{y}t\right)\sin t\sin\left(\frac{2x\alpha^{1/2}}{\varkappa y^2}t^2\right).$$

For $x = 0$ the integral in (53) is calculated exactly:

$$\delta\varphi=0, \qquad \frac{\partial\delta\varphi}{\partial x}=\frac{8\alpha^{1/2}Yy}{\varkappa(y^2+Y^2)^2}.$$

In the limit of large x $[x\alpha^{1/2}/\varkappa y^2 \gg \max(1, Y/y)]$ we have

$$\delta\varphi \approx \varkappa y/4|x|\alpha^{1/2}.$$

In the case of screening, $\lambda \neq 0$ $(\lambda^2 \ll \varkappa^2)$, we find from Eqs. (34), (35), (40) and (41)

$$\delta\Phi=-\frac{\varkappa^2 v}{2}\Delta\mathscr{D}*\rho(x),$$
$$\delta\frac{\partial\varphi}{\partial x}=\varkappa^2\frac{\partial^2}{\partial x\,\partial y}\mathscr{D}*\rho(x), \tag{54}$$

where

$$\mathscr{D}(x,y)=\frac{1}{2\pi(\alpha^*)^{1/2}\varkappa^2}\ln(y^2+\alpha^*x^2)^{1/2}$$

is the solution of the equation $\hat{K}\mathscr{D} = \delta(x,y)$ in the region $x \gg \varkappa/\lambda^2$, $y \gg \lambda^{-1}$, where

$$\hat{K}\approx-\alpha\lambda^2\partial^2/\partial y^2-\varkappa^2\partial^2/\partial x^2, \quad \alpha^*=\alpha\lambda^2/\varkappa^2.$$

Using the boundary condition (42), $\Phi(x, y = 0) \equiv 0$, we find for $\lambda Y \gg 1$:

$$\rho(x)=-\frac{4Y(\alpha^*)^{1/2}}{\lambda(Y^2+\alpha^*x^2)}. \tag{55}$$

The total charge

$$Q=\frac{L_z}{s}\int\rho(x)\,dx=-\frac{4\pi L_z}{\lambda s} \tag{56}$$

does not depend on the length Y, i.e., contrary to the case without screening, only a partial compensation of the dislocation charge $2N$ occurs.

As in the case when screening is absent, the boundary condition $\partial\varphi(x, y = 0)/\partial y \equiv 0$ is satisfied irrespective of the induced charge distribution $\rho(x)$, which can be verified with the help of (54), if we allow for higher derivatives in the operator K. Using (35), we find, in terms of Fourier-components, for $y \to 0$:

$$\delta\frac{\partial\varphi}{\partial y}\propto\int_0^\infty dk_x\,dk_y\frac{\sin(k_x x)\sin(k_y y)k_x k_y\rho(k_x)}{\alpha k_y^4+\lambda^2k_y^2+\varkappa^2k_x^2}$$

$$\to y\int_0^\infty dk_y\,dk_x\frac{k_y^2}{\alpha k_y^4+\lambda^2k_y^2+\varkappa^2k_x^2}k_x\sin(k_x x)\rho(k_x)\to yf(x)\to 0.$$

Neglecting the term αk_y^4 in the denominator, which is valid for $y \gg \lambda^{-1}$, we would find

$$\delta\frac{\partial\varphi}{\partial y}\to g(x)\neq 0$$

as $y \to 0$. Thus, to satisfy the boundary condition for $\varphi(x,y)$, it is necessary to use the solutions (46) which are exact in the region $y \gg \lambda^{-1}$.

The solutions for the fields Φ and φ have the form (49) and (53), where the functions Φ_0 and φ_0 are given by Eqs. (40) and (41). In the distant region $\lambda Y \gg 1$, $y \gg \lambda^{-1}$ and $x \gg (\alpha^*)^{-1/2}\lambda^{-1}$ we get from (54) and (55):

$$\delta\Phi=\frac{\varkappa v\alpha^{1/2}[(Y+y)^2-\alpha^*x^2]}{\lambda^2[(Y+y)^2+\alpha^*x^2]^2}, \tag{57}$$

$$\delta\frac{\partial\varphi}{\partial y}=\frac{4x\alpha^{1/2}(y+Y)}{\lambda[(Y+y)^2+\alpha^*x^2]^2}. \tag{58}$$

At large longitudinal distances we find for $x(\alpha^*)^{1/2} \gg Y,y$:

$$\Phi=\Phi_0+\delta\Phi\approx\frac{\varkappa vY\alpha^{1/2}}{\lambda\alpha^*x^2}\gg\delta\Phi\approx\frac{\varkappa v\alpha^{1/2}}{\lambda^2\alpha^*x^2}.$$

At large transverse distances for $y \gg Y$, $(\alpha^*)^{1/2}x$ we have

$$\Phi\approx-\frac{\varkappa vY}{\lambda y}\gg\delta\Phi\approx\frac{\varkappa v}{\lambda^2y^2}.$$

The similar expressions are found for the function φ. Thus, in the case of screening we can disregard the contribution of the induced charge $\rho(x)$ to the fields φ and Φ in the higher orders, i.e.,

$$\Phi\approx\Phi_0(x, y+Y)-\Phi_0(x, y-Y),$$
$$\varphi\approx\varphi_0(x, y+Y)-\varphi_0(x, y-Y).$$

5. DISLOCATION ENERGY

Let us now calculate the dislocation energy near the surface. It is easy to show that the general expression for the dislocation energy[3,4] does not change in the presence of a charged equipotential, $\Phi_0 = 0$, metallic surface. For a pair of dislocations it has the form

$$W = \frac{L_z}{s} \int_{L_1}^{L_2} \left(v \frac{\partial \varphi}{\partial x} + 2\Phi \right) dy. \tag{59}$$

Substituting the expressions (36), (37), (44), (40), and (41) for the fields Φ and φ into (59), we find the following results valid for the boundary with vacuum (screening is not taken into account).

In the unscreened region $\lambda L_{1,2} \ll 1$ we have

$$W = \frac{\pi \varkappa v \alpha^{1/2}}{2} (Y_2 - Y_1) \frac{L_z}{s}, \quad L_1, L_2 \ll \lambda^{-1}, \tag{60}$$

i.e., the same result as for infinite medium.

In the screened region $\lambda L_{1,2} \gg 1$, $\lambda |L_1 - L_2| \gg 1$

$$W = \frac{\varkappa v \alpha^{1/2}}{2\lambda} \left[2 \ln((Y_2 - Y_1)\lambda) - \ln \frac{(Y_1 + Y_2)^2}{4 Y_1 Y_2} \right]. \tag{61}$$

We have obtained a result of the usual theory of elasticity, corresponding to pair attraction to the surface by image forces.

Let us calculate now the energy of a single dislocation near a lateral metallic surface. Substituting the solutions (49), (50), and (53) into (60), we find in the unscreened region

$$W = \ln 2 \cdot \alpha^{1/2} \varkappa v Y L_z / s < W_0 = {}^1/_2 \pi \alpha^{1/2} \varkappa v Y L_z / s, \tag{62}$$

i.e., we have the law of area conservation with a smaller factor. Thus, the energy of a dislocation with a given charge is numerically smaller under the contact.

In the screened region for $\lambda Y \gg 1$ we find from (40), (41), (57) and (58) only corrections of type Eq. (61) to the energy:

$$W = \left[\frac{\varkappa v \alpha^{1/2}}{\lambda} \ln(Y\lambda) - \frac{v}{2(\alpha^{\cdot})^{1/2} \lambda Y} \right] \frac{L_z}{s}. \tag{63}$$

6. HIGH DENSITIES AND LOW TEMPERATURES: PERIODIC DISLOCATION LATTICE

We have shown that the energy of dislocations located near the surface is lower than their energy in the bulk, i.e., dislocations are attracted to the surface. For a sufficiently high dislocation density near the surface, a periodic structure emerges. Assume, for simplicity, that dislocations are the same distance x_0 apart and have the same depth y_0, i.e., the dislocation lines are at the distance y_0 from a surface which can naturally be regarded as metallic. The energy of a system of N dislocations is

$$W \propto N \int_0^{y_0} \bar{\Phi}\, dy. \tag{64}$$

where $N x_0 = L_x$ is the contact length,

$$\bar{\Phi} = \sum_{-\infty}^{\infty} \Phi(n x_0, y)$$

is the field created by all dislocations on the line $(x = 0, y)$, and Φ is the field of one dislocation with allowance for the induced surface-charge contribution.

Consider, first, an arrangement for which the dislocation fields strongly overlap, i.e., $\varkappa y_0^2 / |x_0| \ll 1$. Using the formulas (51) and (64), we find

$$W \propto N \left[W_0 + \frac{(2\pi)^{1/2}}{8} \frac{\varkappa v y_0^{4}}{\alpha^{1/4}} \left(\frac{\varkappa}{x_0} \right)^{3/2} \right], \tag{65}$$

where W_0 is the energy of an isolated dislocation:

$$W_0 = (\alpha^{1/2} \varkappa v y_0 \ln 2 + C \alpha^{1/2} v), \quad C \sim 1.$$

The second term of the expansion in y_0 in the expression for W_0 is the self-energy of a dislocation line.[3,4]

The functional (65) is minimized for a given electric charge $Q = 2 y_0 N L_z / s$ or a given charge density proportional to $q = y_0 / x_0$. As a result, we have

$$y_0 \propto \frac{1}{\varkappa q^{3/5}}, \quad x_0 = \frac{y_0}{q} \propto \frac{1}{\varkappa q^{8/5}}, \quad \Phi_0 - \mu_0 \propto q^{3/5}, \tag{66}$$

with $\varkappa y_0^2 / x_0 \propto q^{2/5}$, i.e., the condition $\varkappa y_0^2 / x_0 \ll 1$ is satisfied for small q. Thus, dislocations with small charges q are sparse and at a large depth, but their interaction is strong.

When we neglect screening, we assume that two conditions hold: $\lambda y_0 \ll 1$ and $\lambda^2 x / \varkappa \ll 1$. The second condition becomes invalid first, i.e., the dislocation interaction is screened. We find the following constraint: $q \ll (\lambda / \varkappa)^{5/4}$.

Consider the opposite case, when $\varkappa y_0^2 / x_0 \gg 1$. Summation in (64) is performed with the help of the Poisson formula. Using the solutions (38) and (52), we get for $y_0 \gg x_0$:

$$\begin{aligned} \bar{\Phi}(y) = {} & \frac{\pi \varkappa^2 v}{2} \frac{y_0}{x_0} (2y_0 - y) \theta(y_0 - y) + \frac{2}{x_0} \sum_{m=1}^{\infty} \frac{\varkappa v x_0}{4m} \\ & \times \{ \exp[-\delta(y + y_0) m^{1/2}] [\sin(\delta(y + y_0) m^{1/2}) - 2 \sin(\delta y_0 m^{1/2}) \\ & \times (\cos(\delta y m^{1/2}) - \sin(\delta m^{1/2}))] + \exp[-\delta(y - y_0) m^{1/2}] \\ & \times \sin(\delta(y - y_0) m^{1/2}) \}, \end{aligned} \tag{67}$$

where $\delta = (\pi \varkappa / x_0)^{1/2}$.

Summing the series (67), apart from exponentially small terms $\propto \exp(-\varkappa y_0^2 / 4x)$, we find from (64)

$$W \propto L_x \left(\frac{\pi \varkappa^2 v}{3} \frac{y_0^3}{x_0^2} + \frac{\varkappa^{1/2} v}{x_0^{1/2}} \frac{1}{2\pi^{1/2}} \sum_1^{\infty} \frac{1}{m^{3/2}} \right). \tag{68}$$

Minimizing (68) for a given q, we would find the values

$$x_0 \propto 1 / \varkappa q^2, \quad y_0 \propto 1 / \varkappa q, \tag{69}$$

outside the allowed range x_0, $y_0 < \varkappa^{-1}$.

The results (66) and (69) show that for low charge densities ($q \ll 1$) dislocations are sparse, $x_0 \propto q^{-8/5}$, but have a large penetration depth $y_0 \propto q^{-3/5}$. For high charge densities ($q \gg 1$) dislocations are dense and have a small penetration depth: x_0, $y_0 \lesssim \varkappa^{-1}$.

7. CONCLUSION

We have considered the structure of a distorted CDW near a lateral metallic surface. We have shown that charge penetration and electric field screening are realized through the inhomogeneous distribution of solitons and dislocations. We have derived and solved self-consistent equations of elasticity theory for a CDW with topological defects, with accompanying Coulomb fields taken into account. For relatively high temperatures we have found the distributions of the soliton gas density $\rho_s \propto T / y^2$ and the field over the sample depth y. We have also calculated the contact capacitance $C \propto Q$, where Q is the surface charge.

An interesting feature of equilibrium soliton distributions is the invariance $\partial\varphi/\partial y = 0$ of the CDW geometric pahse φ, which determines the observed structural deformations $\propto \cos(2k_F x + \varphi)$. In other words, elastic deformations related to charge polarization at equilibrium and phase discontinuity on solitons are cancelled.

For low temperatures and densities we have thoroughly examined the fields and induced charges created by a single dislocation under a metallic surface. The solution of this problem, in contrast to the contact with vacuum, does not reduce, as usual, to image technique, but requires explicit allowance for the induced electric charge density $\rho(x)$. A dislocation located not deeper than the residual screening length λ^{-1} affects large longitudinal distance x: $x \leqslant \lambda^{-1}$, $x \leqslant \varkappa Y^2$; $|\Phi| \approx \mu_1, \rho(x) \propto 1/s\varkappa Y^2$. Within the screening radius, $\lambda Y < 1$, we have, as in the case of loops in the bulk,[1,2] confinement. A dislocation is attracted with a constant force $F = \mu_i/s$ (per unit length L_z), where $\mu_i > \mu_0$ for the vacuum boundary or in the bulk, and $\mu_i = \mu_1$ for the metallic boundary. An important result is that $\mu_1 < \mu_0$ numerically, i.e., the region under the contact is, in comparison with the rest of the surface, a dislocation potential well.

Another important difference of the region under the contact is that the quasiparticle potential $V \approx \Phi$ has a negative minimum near the dislocation for $y \geqslant Y$. Thus, in contrast to the bulk dislocations, a dislocation can grow owing to injected carriers or solitons accumulated in its vicinity.

When a critical difference $\Phi > \mu_1 \approx \alpha^{1/2}\omega_p$ in CDW and metal potentials is reached, a periodic dislocation structure arises. For small charges near the threshold the dislocations are a large distance x_0 apart and, unexpectedly, at a large depth y_0 [see (69)].

The boundary between the soliton and the dislocation regimes of charge-density and screening of contact potential difference is, probably, of the type of liquid–gas phase transition. Consider the unscreened regime $Y < \lambda^{-1}$ for sufficiently weak Coulomb interaction ($\mu_0 \leqslant \mu_1 < E_s$) and interplanar coupling (see the Introduction). Owing to the area law for their energy ($W \propto N$), the dislocations fix the soliton chemical potential similar to saturated vapor. Therefore the dislocation emergence, like the dew point, is determined by the line $\mu(\rho_s) = \mu_0 - E_s < 0$, $\rho_s \propto d^{-1} e^{\beta\mu}$. In the weak-screening regime, $Y > \lambda^{-1}$, the perimeter law $W \propto N^{1/2} \ln N$ fixes the value $\mu_0 = 0$ for distant dislocations, which, one would think, allows the existence of dislocations for a very low soliton density. However, the screening condition imposes restrictions on the regime of screened dislocations:

$$\lambda/\varkappa \approx (\rho_s l_T)^{1/2} > q^{4/5}.$$

This inequality limits the charge from above and the density or temperature from below.

The general conclusion is that the contact region is a natural generator and accumulator of CDW topological defects, which may serve as nuclei of phase-slippage centers when longitudinal current flows in the sample.

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