Possibility of transition of a Peierls dielectric into the metallic state in a strong electric field

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It is shown that owing to the influence of an external electric field on the gap, a Peierls dielectric should exhibit an appreciable dependence of the dielectric constant on the field and should go over into the metallic phase in sufficiently strong field. The initial premises are discussed for considering the inhomogeneous states that are essential in the region of strong fields and finite temperatures.

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It is known that at $T=0$ a one-dimensional metal is unstable against a lattice restructuring connected with the formation of the dielectric gap (the Peierls transition[1]). This is probably why many known quasi-one-dimensional compounds are insulators (semiconductors).[2] In this article we wish to call attention to the fact that a strong electric field parallel to the easy-conductivity axis can contribute to the stabilization of the metallic phase. This conclusion is a consequence of the thermodynamics of the metal in an electric field. The large values of the dielectric constants of quasi-one-dimensional compounds[3,4] complicate the picture, but are in themselves sources of interesting phenomena which will be discussed below.

We consider a plane-parallel layer of a Peierls dielectric with a surface perpendicular to the one-dimensional chains, placed in a capacitor that produces a field intensity E_0 (Fig. 1). The thermodynamic relation for the free energy per unit volume is

$$dF = EdD/4\pi . \tag{1}$$

In the dielectric (d) phase we have $E=D/\epsilon$, where $\epsilon = \epsilon_{\parallel}$ is the dielectric constant, and by virtue of the geometry of the experiment we have for the electric induction $D=E_0$. Integrating, we get

$$F_d(E_0) = F_d(0) + E_0^2/8\pi\epsilon . \tag{2}$$

In the metallic (m) phase, the field is pushed out of the sample because of the formation of surface charges ($E=0$), and therefore

$$F_m(E_0) = F_m(0) . \tag{3}$$

The difference $F_d(0) - F_m(0)$ is negative because the Peierls phase is favored over the metal phase (we consider for simplicity the case $T=0$). Equating (2) and (3) we obtain the transition field E_c. Assuming that $F_m(0) - F_d(0) \sim \frac{1}{2}N(\epsilon_F)\Delta^2$ (Δ is the gap), we obtain the characteristic value $E_c \sim 10^6$ V/cm. The field in dielectric is weaker in this case because it is attenuated by a factor $\epsilon \sim 10^3$. The usual breakdown mechanisms (see[5]) can therefore turn out to be less effective.

In the Lindhard model, using the strong-coupling approximation,[2] we obtain the value of the static dielectric constant of a one-dimensional dielectric (at $T=0$)

$$\epsilon = 1 + \frac{4\pi e^2}{S}\int_{-\pi/2a}^{\pi/2a}\frac{2dk}{2\pi}\frac{(\partial\phi_k/\partial k)^2}{2\epsilon_k} ,$$

$$\epsilon_k = \sqrt{\Delta^2 + 4b^2\cos^2 ka} , \quad \phi_k = \operatorname{arc\,tg}\left(\frac{\Delta}{2b}\operatorname{tg} ka\right). \tag{4}$$

b is the resonant integral of the transition of the electron between neighboring sites, a is the interatomic distance, and ϵ_k is the dispersion law. The dielectric constant (4) is due to interband transitions and in the limit of weak electron-phonon coupling it takes the form

$$\epsilon = \epsilon_0\left(\frac{4b}{\Delta}\right)^2 , \qquad \epsilon_0 = \frac{e^2a}{12Sb} . \tag{5}$$

Here $4b$ is the total width of the band, S is the cross-section area transverse to the filaments per filament. The energy, with allowance for the electrostatic term $E_0^2/8\pi\epsilon$ takes the form (cf.[2])

$$E = -\frac{\Delta^2}{8\pi b}\ln\frac{e(8b)^2}{\Delta^2} + \frac{\Delta^2}{4\pi b g^2} + Sa\frac{E_0^2}{8\pi\epsilon_0}\left(\frac{\Delta}{4b}\right)^2 . \tag{6}$$

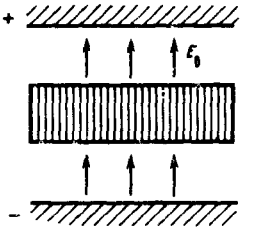

FIG. 1.

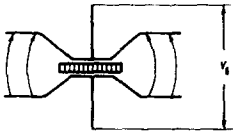

FIG. 2.

Minimizing (6) relative to Δ, we obtain $\Delta = \Delta(E_0)$. Consequently, Δ itself becomes a function of the field. In weak fields we have the estimate

$$\Delta\epsilon/\epsilon \sim (E_0/E_c)^2, \quad E_c \sim e/S. \tag{7}$$

The Peierls transition can be regarded as Bose condensation of phonons with $q = 2k_F$. Denoting the creation operators of the latter by a_0^+ and retaining only these operators in the electron-phonon Hamiltonian, we obtain

$$H_{int} = \lambda(a_0 + a_0^+)\sum_m (a_{2m}^+ a_{2m-1} - a_{2m}^+ a_{2m+1} + \text{H.c.}). \tag{8}$$

By virtue of the Bose condensation, a_0 can be replaced by a c-number

$$a_0 \approx \sqrt{N}\, e^{i\chi}, \tag{9}$$

where $N \gg 1$. An important factor is the presence of the phase χ in (9), which leads to two qualitative effects. Expressing the energy (6) as a function of N and χ, we obtain closed equal-energy curves in phase space (N and χ are canonically conjugate variables). From the quasiclassical quantization rule $\oint N d\chi = 2m(n+\gamma)$ we obtain the discrete spectrum of the excited states and the frequencies of the collective oscillations $\hbar\omega = E_{n+1} - E_n$. This duplicates the results of Lee, Rice, and Anderson[6] for the threshold of the collective mode, which we can regard as a phenomenon analogous to Josephson plasma oscillations in superconductors.[7] Another aspect of the introduction of the phase is connected with the existence of static solutions (solitons), in which the phase varies from 0 to 2π, and which correspond to quantized defects of the homogeneous structure.

A possible way of observing the indicated effect may be to connect a plate of a Peierls dielectric (KCP, TCNQ, and others) in an open cavity resonator of the Fabry-Perot type (Fig. 2) and measuring the changes of the natural frequency when a dc voltage V_0 is applied to the metallic electrode. The scale of the effect in question was indicated above (formula (7)).

A few concluding remarks. We are not concerned here with the metal-dielectric transition observed in vanadium oxides (three-dimensional structures) in[8] (see[9]), nor with the possible nonstationary properties of one-dimensional systems in strong fields.[10,11] The changes due to the finite temperature (due to the screening effect, i.e., to the finite number of carriers in the upper band) and to the role of the "noncommensurability" of the periods of the Peierls structure and of the main lattice ("slipping" of the Peierls phase) will be discussed in another paper.

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