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FAR INFRARED CONDUCTIVITY IN KCP

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Abstract The pinning mechanism based on the $2k_F$-quasi-periodicity of the bromine potential along the chain axis in KCP is used to get the f.i.r. conductivity. Fair agreement with the experimental data is obtained when the phason life-time is included.

INTRODUCTION

The zero frequency of the sliding phase mode is shifted in real quasi-one-dimensional materials towards a non-zero value ω_T which amounts to a finite energy needed to move the CDW in the lattice. As the oscillations of the phase ϕ of the order parameter $\Delta \exp(i\phi)$ induce a dipole momentum a peak develops in the optical conductivity, centered at ω_T. This peak has been detected at low temperatures[1] in the f.i.r. region of the optical conductivity of KCP ($\omega_T \cong 1.9$meV). A further confirmation of the pinned phase mode in KCP has been brought by the inelastic neutron scattering experiments[2] which yielded $\omega_T \cong 2.5$meV, in fair agreement with the optical data.

It has been shown[3] that it seems more realistical to consider the bromine distribution in KCP as being $2k_F$-quasi-modulated along the chain instead of being distributed at random (k_F being the Fermi momentum). A $2k_F$-periodic potential arises this way which, when associated with an extra elastic energy stored by the modulated bromine distribution, allows us to construct a consistent theory of the pinning mechanism in KCP.

The part assigned by this theory to the bromines is essential since they are viewed as inducing the Peierls-Fröhlich transition. A similar attempt has been reported recently.[4] Within the present theory of the pinning in KCP[3] distinction is made between the d.c. gap $2\Delta = 0.11eV$ and the optical one $2\Delta_{op} = 0.2eV$[5], the latter including the strength V of the bromine periodic potential, $\Delta_{op} = \Delta + V$. As this additional interaction is repulsive ($V>0$) the mean field theory predicts a fixed value $\phi = 0$ of the phase of the distortion in the ground state : it means that the hamiltonian has the same reduced symmetry as the ground state has, the broken symmetry is no longer spontaneous but induced and the Goldstone mode (sliding phase mode) is shifted to a non-zero frequency. By means of the aforementioned pinning mechanism the relatively large pinning frequency ω_T is obtained in KCP. With only two fitting parameters, V and λ_i (the coupling strength associated with the bromine extra elastic energy) one can reproduce satisfactorily the distorted spectra of phasons and amplitudons, the distorsion amplitude of the $Pt(CN)_4$ complexes (related to the d.c. gap 2Δ and not to the optical one). The essential features of the optical data are also reproduced when one allows for a finite phason life-time Γ^{-1}.

Microscopic calculations of the f.i.r. properties of the KCP are reported here. They are based on a three-fold extension of the usual theories : (i) $2k_F$-quasi-periodicity of the bromines is assumed along the chain, (ii) the bandwidth cut-off parameter k_c previously introduced into the approach of the giant Kohn anomaly[6] is used and (iii) finite phason life-time Γ^{-1} is allowed for.

DIELECTRIC FUNCTION

Within the bubble approximation of a gauge invariant electromagnetic (transverse) response theory[7] the dielectric function

is given by

$$\varepsilon(\omega) = 1 + \lim_{q\to o} (4\pi e^2/Aq^2)\left[if_{oo}(q,\omega) + \tfrac{1}{2}g_o^2 D_\phi(q,\omega)\cdot f_{o2}(q,\omega)f_{2o}(q,\omega)\right], \quad (1)$$

where long range Coulomb interaction was included (A is the transverse area per chain), g_o is the electron-phonon coupling constant at $2k_F$, $D_\phi(q,\omega)$ is the phason propagator (pinning frequency ω_T and phason life-time Γ^{-1} included) and the f-functions are those usually obtained within the response theory[7]; the only difference here is that the bandwidth cut-off parameter k_c is included. In the f.i.r. region one gets from Eq.(1)

$$\mathrm{Re}\,\varepsilon(\omega) = \varepsilon_\infty(\omega^2 - \omega_L^2)(\omega^2 - \omega_T^2)^{-1},$$
$$\varepsilon_\infty = 1 + \omega_p^2/6\Delta_{op}^2, \quad \omega_p^2 = (8e^2 v_F/A)^{\frac{1}{2}}, \quad (2)$$
$$\omega_L^2 = \omega_T^2 + 1.5\lambda\omega_o^2$$

and the conductivity

$$\mathrm{Re}\,\sigma(\omega)/\sigma_{max} = (2\omega\Gamma)^2\left[(\omega^2 - \bar{\omega}^2)^2 + (2\omega\Gamma)^2\right]^{-1},$$
$$\bar{\omega}^2 = \omega_T^2 + \Gamma^2, \quad (3)$$

where ω_o is the undistorted phonon frequency and $\lambda = 2g_o^2/(\pi v_F\omega_o)$ is the electron-phonon coupling constant (v_F is the Fermi velocity). All the optical data of KCP are satisfactorily reproduced by these equations making use of only three fitting parameters : V, λ_i and Γ. In particular the well known reflectivity and f.i.r. conductivity curves at low temperatures (below the three-dimensional ordering temperature)[1,5] are obtained with Γ of the order of 0.3 - 1meV, values which agree with that extracted from the neutron scattering data (0.5meV).[2] The bandwidth cut-off values k_c agree with the estimations of the width of the Kohn anomaly dip.[2,6] The agreement is expected

to get improved by allowing for an ω -dependence of the Γ parameter.

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