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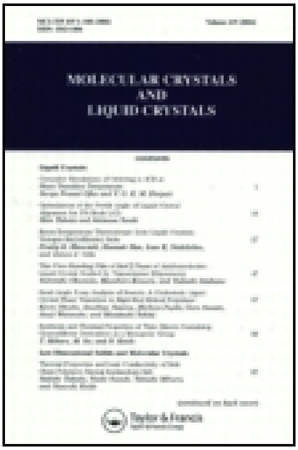

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On the Lattice Excitations in KCP

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ON THE LATTICE EXCITATIONS IN KCP

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Abstract A new mechanism of pinning is put forward in KCP, based on the $2k_F$-quasi-modulated bromine distribution.

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PINNING MECHANISM

The sliding phase mode predicted by the Peierls-Fröhlich theory is pinned in the real quasi-one-dimensional materials mainly by three mechanisms[1]: commensurability of the CDW with the underlying lattice, interchain coupling and impurity effect. The pinning frequency in KCP has been estimated from the f.i.r. conductivity ($\omega_T \cong 1.9$meV)[2] and inelastic neutron scattering experiments ($\omega_T \cong 2.5$meV)[3] at low temperatures.

However, despite the qualitative prediction of the pinned CDW[1] no satisfactory quantitative estimations of the rather large pinning frequency in KCP have been reported until now. The commensurability of the CDW with the underlying lattice is negligible in KCP due to the large value of the commensurability order ($M = 10$).[1] The interchain coupling in this material is also too small[1,4] so as to produce a relatively large pinning frequency, a fact which can straightforwardly be seen from the reduced magnitude of the transverse correlation length ($\cong 50$Å).[3,5] As regards the impurity mechanism of pinning it has been shown[4,6] that the wellknown disruptive effect of the randomly distributed impurities can not be overcome even by the long range Coulomb interaction (although the part played by

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this interaction in KCP is important) and, consequently, the long range ordered CDW state and the high values ($\gtrsim$ 400Å)[3,5] of the correlation length along the chain remain unexplained by this theory when applied to the bromines in KCP (weak pinning case).[4,6] The critical temperature of the Peierls-Fröhlich transition as well as the absence of the transverse dispersion of the phase mode in KCP can not be understood within the theory of the randomly distributed impurities and, in particular, the relatively large values of the correlation length along the chain and pinning frequency obviously can not be corelated by the "domain-size" assumption.

Nevertheless, a deeper look at the sites whereat the bromine and the (additional) water molecule are located in the unit cell[7] as well as at the bromine concentration (0.3 per molecule) seems to support an opposite attitude towards the bromine distribution along the chain. Assuming that the succession of the bromines (B) and (additional) water molecules (W) in the unit cells along the chain is as follows : (BBW)()(BBW)()(BBW)(), where an extra water molecule (W) occupies one out of the three blank spaces, then we have a basic average modulation of wavelength 20c/3, c being the Pt-Pt distance, over which a small disorder is superimposed, brought about by the additional W which comes to fill one out of the three blank spaces. The bromine concentration is 6/20 = 0.3 per molecule and that of the (additional) water is 4/20 = 0.2 per molecule, in agreement with the chemical data. The average modulation of wavelength 20c/3 corresponds to the wavevector $0.3\pi/c = 2k_F$, k_F being the Fermi momentum. The small disorder which arises from the additional W is ineffective to a large extent due, on the one hand, to the low concentration of this W (one to 20 unit cells) and, on the other hand, to the fact that the bromine+water chains do not coincide with the platinum chains, which helps to enhance the three-dimensional effects. Therefore it seems very probable that the bromine distribution along the chain is $2k_F$-quasi-modulated, a fact which might be observed experimentally at low temperatures. The corresponding extra potential ($2k_F$-periodic) and the extra elastic energy stored by the bromines allow us to construct a consistent theory by means of which the long range correlated CDW state in KCP, the pinning frequency, the connection between the distorsion amplitude and the d.c. gap as well as the distinction between this gap and the optical one can be understood.

PINNING FREQUENCY

Adding a $2k_F$-periodic potential of strength V and an extra elastic energy $\Delta^2/\pi v_F \lambda_i$ (Δ being the magnitude of the order parameter along the Pt chain, v_F-Fermi velocity and λ_i a coupling strength related to the bromines) to the well known mean field hamiltonian one obtains the optical gap $\Delta_{op} = \Delta + V$ and an effective phonon coupling strength $\bar{\lambda} = (1/\lambda + 1/\lambda_i)^{-1}$. Introducing the distortion amplitude $u_0 = 0.025$Å[6,7] into

$$u_0 = (2\Delta/\omega_0)(c/\pi v_F \lambda M)^{\frac{1}{2}},$$

where ω_0 is the frequency of the undistorted phonons and M the mass of $Pt(CN)_4$ complex, we get at once 2Δ = o.11eV which is exactly the experimental value of the d.c. gap.[8] The coupling strength λ is about 0.45 in fair agreement with other estimations. It follows that the d.c. gap is associated with the Pt distortion amplitude while the optical gap $2\Delta_{op} = 0.2$eV includes the bromine contribution V. The distorted phonon spectrum near $2k_F$ (amplitodons and phasons)[3] is well reproduced by taking appropriate values of the fitting parameter λ_i. In particular the pinning frquency is given by

$$\omega_T^2 = \omega_0^2(1 - \lambda\Delta/\bar{\lambda}\Delta_{op}).$$

Below 80K we get $\lambda_i > 0.55$ which means that the present pinning mechanism is effective when the CDW state in KCP is clear-

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ly established. For $\lambda_i < 0.55$ we get a soft mode suggesting that a pseudo-gap regime dominates.

REFERENCES

1. P. A. Lee, T. M. Rice and P. W. Anderson, Solid State Commun. 14, 703 (1974).
2. P. Brüesch, S. Strässler and H. R. Zeller, Phys. Rev. B12, 219 (1975).
3. K. Carneiro, G. Shirane, S. A. Werner and S. Kaiser, Phys. Rev. B13, 4258 (1976).
4. H. Fukuyama, J. Phys. Soc. Jpn. 45, 1266 (1978).
5. J. W. Lynn, M. Iizumi, G. Shirane, S. A. Werner and R. B. Saillant, Phys. Rev. B12, 1154 (1975).
6. P. A. Lee and H. Fukuyama, Phys. Rev. B17, 542 (1978).
7. C. F. Eagen, S. A. Werner and R. B. Saillant, Phys. Rev. B12, 2036 (1975).
8. G. A. Toombs, Phys. Rep. 40, 181 (1978).

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