Effect of phonon dispersion on mobility of strongly-coupled polarons in one-dimensional and three-dimensional crystals

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The mobility of strongly-coupled polarons is investigated in conducting polymers and other quasi-one-dimensional conductors. Interaction of electrons with optical phonons is treated, taking into account dispersion of the optical phonons; the mobility of polarons is also analyzed in three-dimensional crystals, again including in the analysis optical phonon dispersion. The spectrum of acoustic polarons is studied in one-dimensional conductors.

1. INTRODUCTION

Recently there has been a notable growth in interest in the theory of one-dimensional polarons,[6–17] in conjunction with intensive experimental investigation of the electric, magnetic and optical properties of quasi-one-dimensional organic semiconductors and conducting polymers[1–4] with strong electron-phonon coupling.[5–8] The foundation of this theory was laid in the papers of Rashba[18] and Holstein[19] (see also the review in Ref. 20). This new interest is a consequence both of the interesting experimental data on the properties of polarons in conducting polymers[1–8,21] and of the possibility of finding exact solutions to a whole range of polaron problems.[9–17] Among the most interesting theoretical results obtained in this area, we should mention results on autolocalization of an electron in a Peierls dielectric,[6–8] on bound states of a polaron plus phonons,[12] on the spectra of acoustic polarons[9,14–16] and on bound states of two polarons.[8,13]

The great progress made in the theory of such states[6–17] allow us to explain a number of important experimental results related to magnetic and optical properties of polyacetylene $(\mathrm{CH})_x$ [22] and other conducting polymers[1–4] by invoking polaron and soliton models.[6–8] At this time, the mobility μ has not been calculated, nor has its high value ($\mu \sim 10$–10^2 cm^2/V-sec) in $(\mathrm{CH})_x$ [1–4,23,24]) been explained; note that μ can reach values $\sim 10^4$–10^5 cm^2/V-sec in polydiacetylene (PDA).[21] Some estimates for μ were made in Refs. 11, 15–17; however, as we show below, they are qualitative in character and have limited ranges of applicability.

The effective dimensionless constant α which characterizes the interaction of electrons with phonons in polymers of polyacetylene type is fairly large: $\alpha \approx 4$–5,[25,26] while in polydiacetylene it can reach 12.[21] Therefore, the strong-coupling approximation $\alpha \gg 1$ is applicable in these compounds, a situation which is encountered relatively rarely in three-dimensional semiconductors and ionic crystals. This is related to the fact that the criterion for strong coupling in the one-dimensional case is $\alpha > 2$, which is much weaker than the criterion $\alpha > 6$ in the three-dimensional case.[20]

In the present paper, the mobility μ is calculated for strongly-coupled polarons in one-dimensional conductors, and also in three-dimensional ionic crystals. The interaction of electrons with optical phonons is investigated, along with the energy spectrum $\varepsilon(p)$ for one-dimensional strongly-coupled acoustic polarons; this spectrum possess a characteristic saturation velocity $v(p)$ which for large momenta $p \to \infty$ is close to the sound velocity s, a feature which is typical of all acoustic polarons[27,28] ("condensons" in the terminology of Deigen and Pekar[29]). A similar saturation effect in the velocity of current carriers is observed in a number of conducting polymers,[21,30] molecular crystals and other organic compounds.[31–35] The asymptotic behavior of $\varepsilon(p)$ and $v(p)$ for $p \gg \alpha^2 ms$ (m—electron mass) in the case of three dimensional piezopolarons was evaluated by Volovik and Edel'shtein[27]:

$$\begin{aligned} \varepsilon(p) &\approx sp\biggl(1 - \frac{1}{6}\biggl(\frac{\alpha^2 ms}{p}\ln^2\frac{p}{\alpha^2 ms}\biggr)\biggr)\biggr], \\ v(p) &\approx s\biggl(1 - \frac{1}{3}\frac{\alpha^2 ms}{p}\ln\biggl(\frac{p}{\alpha^2 ms}\biggr)\biggr). \end{aligned} \tag{1}$$

In the one-dimensional case the spectrum of an acoustic polaron in the presence of a deformation interaction with one-dimensional acoustic phonons was evaluated by Whitfield and Shaw.[14]

The correct general approach to the mobility problem for strongly-coupled polarons in three-dimensional systems was developed in the papers of Volovik, Mel'nikov and Edel'shtein.[36–38] In the present paper, this method is used to calculate the polaron mobility in one-dimensional systems. As will be shown below, in calculating μ for a one-dimensional system it is necessary to take into account the dispersion of optical phonons, which usually is not considered in polaron theories.[20]

This effect also turns out to be extremely important in the case of three-dimensional crystals, where taking into account phonon dispersion significantly simplifies the calculation of μ and leads to a marked change in the low-temperature asymptotic behavior of $\mu(T)$ in comparison with the results of Volovik, Mel'nikov and Edel'shtein[38]:

$$\begin{aligned} \mu(T) &= \gamma_0\mu_0 n_0(T), \qquad \mu_0 = \frac{e}{m\omega_0\alpha^2}, \\ n_0(T) &= \frac{T}{\omega_0}e^{\omega_0/T}, \qquad \gamma_0 \sim 1, \end{aligned} \tag{2}$$

where ω_0 is the phonon frequency.

2. INTERACTION WITH OPTICAL PHONONS

The Hamiltonian for the interaction of electrons with phonons in units $\hbar = m = 1$ takes the form

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$$H=-\frac{1}{2}\frac{\partial^2}{\partial x^2}+\sum_{\mathbf{k}} V_{\mathbf{k}}e^{ik_x x}Q_{\mathbf{k}}+\frac{1}{2}\sum_{\mathbf{k}}(\omega_{\mathbf{k}}\omega_{-\mathbf{k}}Q_{\mathbf{k}}Q_{-\mathbf{k}}+P_{\mathbf{k}}P_{-\mathbf{k}}), \tag{3}$$

where $Q_{\mathbf{k}}$ is a phonon coordinate and $P_{\mathbf{k}} = -i\partial/\partial Q_{\mathbf{k}}$ is a quantity which is canonically conjugate to $Q_{\mathbf{k}}$, and which plays the role of a momentum. An analysis of experimental data on lattice heat capacities[39] shows that both one- and three-dimensional modes are present in one-dimensional polymer chains; hence the sum over **k** in the Hamiltonian (3) is three-dimensional.

In this section we will investigate the interaction between electrons and optical phonons in quasi-one-dimensional organic compounds.[1–4] There are two basic types of optical phonon modes in the vibrational spectra of such systems[5,40]: intramolecular vibrations which have very small dispersion $\Delta(\mathbf{k}) \ll \omega_{\mathbf{k}} \approx \omega_0$, and intermolecular vibrations which possess significant dispersion $\omega_0(k_x)$ along the chains. Since in the continuum approximation which is usually employed in polaron theories[20] the quantity Δk_x is much smaller than the Bragg momentum k_B, at low temperatures we can make use of a quadratic expansion for $\omega_0(k_x)$ near its minimum, which can be attained at $k_x = k_0 \sim k_B$ [41]

$$\omega_0(k_x)=\omega_0+(k_x-k_0)^2/M_0. \tag{4}$$

In the case of intramolecular modes with very small dispersion $\Delta(\mathbf{k})$, we can neglect the dependence of ω_0 on k_x by virtue of the smallness of k_x compared to k_B and for $T \gtrsim \Delta$ take into account only the transverse dispersion $\Delta(\mathbf{k}_\perp)$. For the simplest case,[41] which gives a good description of the phonon spectrum in organic compounds,[42] this spectrum takes the form

$$\omega_0(\mathbf{k})=\omega_0+\Delta_\perp(\cos k_y+\cos k_z), \quad \Delta_\perp \ll \omega_0. \tag{5}$$

Here the transverse periods of the lattice satisfy $a_y = a_z = 1$, while the quantity $\Delta_\perp$ can have either sign.

The effective constant $V_{\mathbf{k}}$ depends weakly on **k** for the case of non-polar interactions, and is connected with α (in units in which $\omega_0 = 1$) by the relation

$$V_{\mathbf{k}}=(2\alpha)^{1/2}. \tag{6}$$

For the case of polar interactions, which can occur in ion-radical compounds such as TCNQ salts,[14] $V_{\mathbf{k}}$ has a singularity at small k [20,43]:

$$V_{\mathbf{k}}=k^{-1}(2^{3/2}\pi\alpha)^{1/2}, \quad 2^{1/2}\alpha=e^2(\hat{\varepsilon}_\infty^{-1}-\hat{\varepsilon}_0^{-1})=\tilde{e}^2. \tag{7}$$

Here and henceforth we set the crystal volume $\Omega = 1$; $\hat{\varepsilon}_0, \hat{\varepsilon}_\infty$ are the dielectric permittivities at low and high frequencies.

In all cases, the function $\omega_0(\mathbf{k})$ is slowly varying for $k_x \ll k_B$, and we can neglect its **k**-dependence in calculating the polaron spectrum. As was shown by Pekar,[43] in the strong-coupling limit $\alpha \gg 1$ the effective number of phonons participating in the creation of a polaron is given by $N \sim \alpha^2 \gg 1$, so that to lowest order in α^{-1} the phonons can be treated classically. Minimizing the Hamiltonian H in (3) with respect to $Q_{\mathbf{k}}$, we obtain

$$Q_{\mathbf{k}}=Q_{\mathbf{k}}^0=v_{00}(\mathbf{k})\,(\omega_{\mathbf{k}}\omega_{-\mathbf{k}})^{-1},$$

$$v_{nm}(\mathbf{k})=V_{\mathbf{k}}\int dx\, \psi_n^*(x)\,e^{ik_x x}\psi_m(x). \tag{8}$$

Here, $\psi_n(x)$ are the wave eigenfunctions of an electron in the polaron well, which are determined by the minimum of the Hamiltonian for $Q_{\mathbf{k}} = Q_{\mathbf{k}}^0$ (8), while for the corresponding eigenvalues of an electron in the well we find that $\varepsilon_n \sim \alpha^2 \gg 1$.[12,20,36–38,43] The renormalization of the polaron mass M^* is determined from the equilibrium of $Q_{\mathbf{k}}^0$, and takes the form[12,20,36–38,43]

$$M^*=\sum_{\mathbf{k}} k_x^2 Q_{\mathbf{k}}^0 Q_{-\mathbf{k}}^0. \tag{9}$$

For the case of the contact interaction (6), the ground state of H_0 and the quantities ε_n, $\psi_n(\xi)$ in units $\xi = \alpha x$ and $\varepsilon_n = \alpha^2\tilde{\varepsilon}_n$ take the form[9–12,18–20];

$$H_0={}^1/_2\alpha^2\int d\xi[(\partial\psi_0/\partial\xi)^2-2\psi_0^4]=-{}^1/_6\alpha^2,$$

$$[-d^2/d\xi^2-4\psi_0^2]\psi_n=\tilde{\varepsilon}_n\psi_n, \tag{10}$$

where

$$\psi_0(\xi)=(2^{1/2}\operatorname{ch}\xi)^{-1}, \quad \tilde{\varepsilon}_0=-1, \quad \varphi_{\tilde{q}}(\xi)=e^{i\tilde{q}\xi} \times(th\xi-i\tilde{q})/(1-i\tilde{q}), \quad \tilde{\varepsilon}_{\tilde{q}}=\tilde{q}^2. \tag{11}$$

In this case there is only one level ε_0 in the polaron well, and the continuous-spectrum wave function $\psi_{\tilde{q}}(\xi)$ contains no scattered wave. This is connected with the reflectionless character of the potential $4\psi_0^2(\xi) = 2\operatorname{ch}^{-2}(\xi)$.[44] The quantities $v_{0q}(k)$ have the form

$$v_{0q}(\mathbf{k})=i\pi\tilde{k}_xV_{\mathbf{k}}/2^{1/2}(1-i\tilde{q})\operatorname{ch}[\pi(\tilde{k}_x+\tilde{q})/2],$$
$$v_{00}(\mathbf{k})=\pi\tilde{k}_xV_{\mathbf{k}}/2\operatorname{sh}(\pi\tilde{k}_x/2), \quad k_x=\tilde{k}_x\alpha, \quad q=\tilde{q}\alpha. \tag{12}$$

The quantities $M^* = 8\alpha^4/15$ and $H_0 = -\alpha^2/6$ contain numerical coefficients which are larger than their analogues in the three-dimensional case,[20,43] for which $M^* \approx 0.023\alpha^4$ and $H_0 \approx -0.11\alpha^2$ [here we must also take into account the factor $2^{1/2}$, introduced for convenience into the definition of α, (6)]. From the formulae obtained for H_0 and M^* it follows that in the one-dimensional case the region of applicability of the strong-coupling approximation begins at $\alpha > 2$ and not at $\alpha > 6$ as in the three-dimensional case.[20]

3. SCATTERING OF POLARONS

Calculation of the mobility μ is one of the most difficult problems in polaron theory (see the review in Ref. 20). The correct method of solving it was developed by Volovik, Mel'nikov, and Edel'shtein.[36–38] In their papers, with the help of either the transformations of Bogolyubov and Tyablikov[45] and Lee, Low, and Pines[46] or the Feynman path integral method,[47] they carried out a separation of the center-of-gravity coordinate of the polaron in the Hamiltonian and derived terms which describe its scattering. For small velocities $v \ll \alpha^{-1}$ and neglecting recoil effects, the effective Hamiltonian which describes phonon-polaron scattering takes the form[36–38]

$$H=H_0+\frac{p^2}{2M^*}+\sum_{\mathbf{k}}\tilde{\omega}_{\mathbf{k}}\left(b_{\mathbf{k}}^+b_{\mathbf{k}}+\frac{1}{2}\right)+\frac{1}{2}\sum_{\mathbf{k},\mathbf{k}'}V_{\mathbf{k}\mathbf{k}'}(b_{\mathbf{k}}^++b_{-\mathbf{k}})(b_{-\mathbf{k}'}^++b_{\mathbf{k}'}). \tag{13}$$

Here $\widetilde{\omega}_{\mathbf{k}} = \omega_{\mathbf{k}} - \mathbf{kv}$, $\mathbf{v} = \mathbf{p}/M^*$ is the polaron velocity; the Born amplitude for two-phonon scattering $V_{\mathbf{kk}'}$ is expressed in terms of the quantities $v_{nm}(\mathbf{k})$ given in Eq. (8) by

$$(\omega_{\mathbf{k}}\omega_{-\mathbf{k}})^{1/2}V_{\mathbf{kk}'} = \sum_n \frac{v_{0n}(\mathbf{k})\,v_{n0}(-\mathbf{k}')}{\varepsilon_0-\varepsilon_n}. \tag{14}$$

The Doppler shift in the phonon frequencies $\omega_{\mathbf{k}} \to \widetilde{\omega}_{\mathbf{k}}$ is caused by the transformation to the center-of-gravity system of the polaron. It can be included in the original Hamiltonian (3) by a transformation to a comoving reference frame moving with velocity v. For values of $v \sim \alpha^{-1} \ll 1$ which are not too small, this leads to a dependence of ε_n and M^* on velocity. This dependence was investigated by Davydov and Enol'ski for the case of a three-dimensional ionic crystal.

The case of dispersionless optical phonons $\omega_{\mathbf{k}} = \omega_0$ was investigated in Refs. 36–38; however, the derivation of the Hamiltonian (13) does not depend on this, as follows from analogous results on the piezopolaron.[36]

In the Hamiltonian (13) terms have been eliminated which describe one-phonon emission and absorption processes. For temperatures $T \ll \alpha^2$ these processes are accompanied by large momentum transfers $k_x \gg \alpha [k_x \sim M^{*1/2} \sim \alpha^2$ for $T \lesssim 1$ and $k_x \sim (M^*/T)^{1/2} \gg \alpha$ for $1 \lesssim T \ll \alpha^2]$. Therefore they give an exponentially small contribution to the amplitude of one-photon scattering

$$W^0(p,k_x) = v_{00}(\mathbf{k})/\widetilde{\omega}_{\mathbf{k}} \propto \exp(-c_0 k_x/\alpha), \quad c_0 \sim 1$$

and can be discarded.[36,37] In the case of the contact interaction (6) $c_0 = \pi/2$ and therefore the probability of one-phonon processes $|W^0|^2$ contains a numerically small factor $\sim 10^{-3}$ even for $\alpha = 2$. Therefore, for all $\alpha > 2$ we can limit ourselves to terms quadratic in the phonon operators $b_{\mathbf{k}}$, $b_{\mathbf{k}}^+$ for the Hamiltonian (13), which describe "Compton-like" scattering processes. The equation for the full amplitude $W_{k_xk'_x}$ for such phonon scattering processes by the heavy polaron has the form[36–38]

$$W_{k_xk_x'} = V_{k_xk_x'} - \sum_{k_x''} V_{k_xk_x''} \frac{2\widetilde{\omega}_{k_x''}}{\widetilde{\omega}^2_{k_x'} - \widetilde{\omega}^2_{k_x''} + i0} W_{k_x''k_x'}. \tag{15}$$

For $T < 1$ the mobility μ is determined by a kinetic equation, which has the Fokker-Planck form due to the large polaron mass M^* and small momentum transfers $k_x \ll p \sim (M^*T)^{1/2}$ (Refs. 36–38):

$$eE\frac{\partial f}{\partial p} = \frac{\partial}{\partial p}\left(Af + B\frac{\partial f}{\partial p}\right), \quad A = Bv/T. \tag{16}$$

The coefficient B is expressed through the amplitude $W_{k_xk'_x}$ and the Planck form of the phonon occupation number $N_{\mathbf{k}}$ ($N_{\mathbf{k}} \sim \exp(-1/T)$ for $T < 1$):

$$B = \pi \sum_{\mathbf{k},\mathbf{k}'} N_{\mathbf{k}}(N_{\mathbf{k}'}+1)\,|W_{k_xk'_x}|^2 (k_x-k_x')^2 \delta(\widetilde{\omega}_{\mathbf{k}} - \widetilde{\omega}_{\mathbf{k}'}). \tag{17}$$

The mobility μ in weak fields $E \ll E_0 \sim Bp^3$ is determined by the quantity B according to $\mu = eT/B$.

4. POLARON MOBILITY IN ONE-DIMENSIONAL CONDUCTORS

The basic mechanism of interaction between electrons and optical phonons in conducting polymers is the contact interaction (6). In the case of intermolecular vibrations (4) the quantity $M_0 \sim 10\text{–}10^2 m$[42] is small compared to $M^* \sim 10^2 m$ for $\alpha > 3$. Therefore for low temperatures $T \ll 1$ the magnitude of thermal-induced fluctuations in the phonon momentum $\Delta k_T \sim (TM_0)^{1/2}$ is small compared to the polaron momentum $p \sim (TM^*)^{1/2}$. This ensures the correctness of the Fokker-Planck expansion (16). In the case $k_0 \sim k_B$ we can make use of the asymptotic expansion[38] for $V_{k_xk'_x}$ at large momenta $k_x, k'_x \approx k_0 \gg \alpha$:

$$V_{k_xk'_x} \approx \frac{4\alpha}{k_x^2}(\psi_0^2)_{k_x-k'_x}\left(1 - 2\frac{k_x-k_x'}{k_x}\right), \quad k_x-k_x' \sim \alpha \ll k_x, k_x'. \tag{18}$$

Neglecting terms $\Delta k_x v \ll \Delta k_x^2/M_0$ in $\widetilde{\omega}_0(k_x)$, we reduce (15) to an equation for elastic scattering[49] of quantized particles with effective mass $M_0/2$ in a potential $U(\xi) = [2\psi_0(\xi)/k_0]^2$. This Schroedinger equation with $\psi_0(\xi)$ given by (11) can be solved exactly,[44] and $W_{k_xk'_x}$ for $k'_x = M_0 v - k_x \approx -k_x$ has the form

$$W_{k_x,-k_x} = (1 + \operatorname{sh}^2 \pi\tilde{k}_x/\operatorname{ch}^2\varkappa)^{-1}, \quad \varkappa = {}^1/_2\pi(-1+16M_0/k_0^2)^{1/2} \sim 1. \tag{19}$$

The mobility $\mu(T) = \mu_0\gamma n(T)$ for $T \ll T_0 = \alpha^2/M_0 \ll 1$ is determined in the usual units by the relations

$$\gamma = 2\pi(\alpha m/M_0)^2, \quad n(T) = e^{\omega_0/T}, \quad \mu_0 = e/m\alpha^2\omega_0. \tag{20}$$

It contains the small parameter $\alpha m/M_0 \ll 1$ and differs from expression (2) by a pre-exponential temperature-dependent factor in the three-dimensional case. In the temperature regime $T_0 \ll T \ll 1$ the quantity μ is described by formula (2), while the numerical coefficient γ_0 depends on the parameter $\varkappa \sim 1$ (19):

$$\gamma_0 = \pi^3/4f_1(\varkappa), \quad f_1(\varkappa) = \operatorname{ch}^4\varkappa \int_0^\infty k\,dk(\operatorname{ch}2k + \operatorname{ch}2\varkappa)^{-1}. \tag{21}$$

For $\varkappa = 0$, we have $f_1(0) \approx 0.073$ and $\gamma_0 \approx 106$, while for $\varkappa \gg 1$ we have $f_1(\varkappa) \approx \varkappa^2/8$ and $\gamma_0 \approx 2\pi^3/\varkappa^2$. The condition $T_0 \ll 1$ is not restrictive, and is necessary only to determine the numerical coefficients. Therefore in real systems with $\alpha = 5$ and $M_0 = 50m$, the quantity $T_0 = 0.5$ is not too small and we can assume it is of order unity. For these values of the parameters $T \sim T_0 \sim \omega_0$, Eq. (21) for $k_0^2 = M_0\omega_0$ gives $\mu \sim \mu_0 \sim 10^2$ cm²/V-sec, while Eq. (20) gives a smaller estimate—$\mu \sim 0.1\mu_0 \sim 10$ cm²/V-sec. The quantity M_0 was estimated for the values $\alpha = 5$, $\omega_0 = 0.01$ eV and $m = 0.1m_0$ (m_0 is the free electron mass) appropriate to $(\mathrm{CH})_x$ (Ref. 25).

In the case $k_0 = 0$, the characteristic values $k_x, k'_x \lesssim \alpha$ for $T \lesssim T_0$, and we cannot use the asymptotic expansion (18). This complicates the solution of the scattering problem due to the nonlocal potential $U(\xi,\xi')$ whose Fourier transform is $V_{k_xk'_x}$ (14). Therefore, in order to calculate μ for $T \ll T_0$ we make use of a simpler method to solve equation (15), analogous to the procedure used by Volovik and Edel'shtein[36] for the piezopolaron problem.

For $T \ll T_0$ the thermal momenta k_x, k'_x for phonons are small compared to $k''_x \sim \alpha$, and to lowest order in these small quantities we have $\widetilde{\omega}_{k'_x} \approx 1$. We use the expansion (14) of $V_{k_xk'_x}$ for $\tilde{k}_x, \tilde{k}'_x \ll 1$ in this region,

$$V_{k_x k_x'} \approx \frac{\pi}{\alpha} \tilde{k}_x \tilde{k}_x' C_0,$$

$$C_0 = 4\int_0^\infty d\tilde{q}\,(1+\tilde{q}^2)^{-2}(1+\operatorname{ch}\pi\tilde{q})^{-1} \approx 0.888, \tag{22}$$

and the well-known identities which connect $V_{k_x k_x'}$ and $Q^0_{k_x'}$ (Refs. 36, 45):

$$\sum_{k_x'} [\omega_{k_x}\omega_{-k_x'}\delta_{k_x k_x'} + 2(\omega_{k_x}\omega_{-k_x'})^{1/2} V_{k_x k_x'}] k_x' Q^0_{k_x'} = 0, \tag{23}$$

to obtain the following solution for $W_{k_x k_x'}$ to lowest order in $T/T_0 \ll 1$:

$$W_{k_x k_x'} = 2\tilde{k}_x \tilde{k}_x' (Q^0_{k_x}/Q_0^0) \frac{\tilde{k}_x^2}{M_0} \frac{\pi C_0}{\alpha}. \tag{24}$$

Substituting the solution (24) into equation (15) reduces its right-hand side to zero to lowest order in T/T_0; its left side is of the same order as a consequence of the conditions $k_x^2/M_0 \sim T \ll T_0 \ll 1$. Using Eqs. (17), (24) we obtain the following expression for μ:

$$\mu = \mu_0 \gamma n(T), \quad \gamma = (6\pi C_0)^{-1}(\alpha^2 m/M_0)^4, \quad n(T) = (\omega_0/T)^4 e^{\omega_0/T}. \tag{25}$$

For the same parameter values and $T \sim \omega_0$ we obtain the somewhat smaller estimate $\mu \sim 10^{-2}\mu_0 \sim 1$ cm²/V-sec. It is necessary to take into account the fact that, due to the presence of the exponential factor $e^{\omega_0/T}$ and the temperature-dependent coefficient in Eq. (25), this estimate will increase rapidly for $T < \omega_0$; for $T = \omega_0/2$ it gives $\mu \sim 0.1\mu_0 \sim 10$ cm²/V-sec.

In the case of small longitudinal dispersion (5) we can make use of the method employed in Ref. 38 for dispersionless optical phonons. In the integrals over k_x, k_x', (17), as will be shown below, large $k_x, k_x' \gg \alpha$ are present with small transfer $(k_x - k_x') \sim \alpha$, and we can use the asymptotic expansion (18) for $V_{k_x k_x'}$. Carrying out a Fourier transform in $\tilde{k}_x - \tilde{k}_x'$ in equation (15) and introducing the corresponding variables $\tilde{x}$ and function $\tilde{g}(\tilde{x}, k_x')$,

$$-i\int_{\tilde{x}}^\infty W(\tilde{x}', \tilde{k}_x')\,d\tilde{x}' = |v|[1 - \tilde{g}(\tilde{x}, \tilde{k}_x')], \tag{26}$$

we obtain in the units $\alpha = 1$ [cf. Eq. (11)] the equation

$$-i\frac{\partial}{\partial\tilde{x}}\tilde{g}(\tilde{x}, \tilde{k}_x') = \frac{1}{v} V\left(\tilde{x}, \tilde{k}_x' - i\frac{\partial}{\partial\tilde{x}}\right)\tilde{g}(\tilde{x}, \tilde{k}_x'),$$

$$\tilde{g}(+\infty, \tilde{k}_x') = 1. \tag{27}$$

The quantity B in (17) is connected with $\tilde{g}$ by the relation

$$B = \frac{\Delta_\perp^2}{v} e^{-\omega_0/T} \int_{-\infty}^\infty \frac{d\tilde{k}_x'}{2\pi} |1 - \tilde{g}(-\infty, \tilde{k}_x')|^2. \tag{28}$$

Separating the modulus and phase of the function $\tilde{g}$,

$$\tilde{g}(\tilde{x}, \tilde{k}_x') = a(\tilde{x}, \tilde{k}_x')\exp\{i|\tilde{k}_x'|\chi(\tilde{x}, \tilde{k}_x')\}, \tag{29}$$

and using the asymptotic expression (18) for $V(\tilde{x}, \tilde{k}_x' - i\partial/\partial\tilde{x})$, we obtain the following equation for a and χ

$$\frac{\partial\chi}{\partial\tilde{x}}\left(1 + \frac{\partial\chi}{\partial\tilde{x}}\right)^2 = \zeta\psi_0^2(\tilde{x}), \quad \zeta = 4/(\alpha^2|v|\,|\tilde{k}_x'|^3) \sim 1, \tag{30}$$

$$(1-\eta)\frac{\partial}{\partial\tilde{x}}\ln a = \frac{1}{2}\frac{\partial\eta}{\partial\tilde{x}}, \quad \eta = -4\psi_0^2(\tilde{x})\zeta\left(1 + \frac{\partial\chi}{\partial\tilde{x}}\right)^{-3}. \tag{31}$$

From equation (31) it follows that $a(+\infty, \tilde{k}_x') = a(-\infty, \tilde{k}_x') = 1$ and the mobility μ are expressed entirely in terms of the function χ:

$$\mu = \mu_0\gamma n(T), \quad \gamma = \left(\frac{\alpha^4 m}{M^*}\right)\left(\frac{\omega_0}{\alpha\Delta_\perp}\right)^2 \frac{3\pi}{C_1},$$

$$n(T) = n_0(T)\frac{T}{\omega_0}, \tag{32}$$

where

$$C_1 = \int_0^\infty \frac{d\zeta}{\zeta^2}\chi^2(\zeta), \quad \chi(\zeta) = \chi(-\infty, \zeta), \quad \chi(+\infty, \zeta) = 0. \tag{33}$$

The function $\chi(\zeta)$ is found from equation (30):

$$\chi(\zeta) = \frac{1}{3}\int_{-\infty}^\infty d\tilde{x}\,[z_1^{1/3} + z_1^{-1/3} - 2], \quad z_1 = 1 + z_0 + (z_0(z_0+2))^{1/2},$$

$$z_0 = \frac{54\zeta}{\operatorname{ch}^2\tilde{x}}. \tag{34}$$

For $\zeta \ll 1$ the function $\chi(\zeta) \propto \zeta$, while for $\zeta \gg 1$ it is proportional to $\zeta^{1/3}$. The value of the numerical coefficient $C_1 \approx 21.5$ determines the value of γ in formula (32). Along with numerical factors, γ contains the large nonnumerical parameter $(\omega_0/\alpha\Delta_\perp)^2 \gg 1$. This is related to the fact that for very small values of the dispersion $\Delta_\perp \to 0$, the forward scattering in one-dimensional systems is purely elastic and gives no contribution to the mobility μ. Its value in this limiting case is determined by the exponentially small backward scattering, $\mu^{-1} \propto e^{-2\pi p/\alpha} \ll 1$ for $T \gg \alpha^{-2}$. In real systems, the quantity $\Delta_\perp \sim 0.1\omega_0$ and the parameter $(\omega_0/\alpha\Delta_\perp)^2$ are not very large. Therefore, for $\alpha = 5$ we have $\gamma \sim 1$ and for $T \sim \omega_0$ the mobility satisfies $\mu \sim \mu_0 \sim 10^2$ cm²/V-sec.

For weak dispersion, the characteristic $k_x \sim \alpha T^{-1/6}$ is small compared to $p \sim \alpha^2 T^{1/2}$ for $\alpha^{-3/2} \ll T \ll 1$. Because of these small powers of T the region of applicability of results in these limits is appreciably reduced. In connection with this it is necessary to emphasize the wider region of applicability of Eqs. (20), (21), (25). We remark that estimates of the value of μ based on Eqs. (20), (21), (25), (32) give reasonable values of mobility which agree with experiments on $(\mathrm{CH})_x$.[1–4,23,24] This confirms the correctness of the model used to describe the kinetics of electrons in conducting polymers.

In conclusion, we note that an estimate of the contribution of one-phonon emission and absorption processes to the mobility μ in the absence of phonon dispersion was made by Holstein.[11] This estimate coincides with our results for these processes and leads to $\mu \propto e^{\pi\alpha}$. These processes, however, can only play a significant role when $\Delta_\perp < \alpha^{-1}e^{-\pi\alpha/2}$, which even for $\alpha > 3$ imposes too strong a limitation on the quantity $\Delta_\perp$, and which is in poor agreement with estimates of this parameter in real quasi-one-dimensional conductors.[5,6,25,40,42]

We remark that for low temperatures $T < \omega_0$ the value of the dispersion $\Delta_\perp$ is assumed to be rather large compared to the probability of polaron scattering per unit time $\tau^{-1} \sim T^2/Bv^2 \ll \Delta_\perp$. This ensures enough inelasticity in the scattering to eliminate effects of localization for electron scattering by dispersionless phonons.[50,51]

5. POLAR INTERACTIONS

The polar interaction (7) is apparently absent in conducting polymers; however, it can arise in ion-radical compounds similar to the TCNQ salts.[1-4]

An estimate of the quantity $V_{\mathbf{kk}'}$ in this case give $V_{\mathbf{kk}'} \lesssim \alpha^{-2} \ll 1$ according to Eqs. (8) and (14), and the integral terms in Eq. (15) turn out to be small, at least when $T \gg \alpha^{-2}$. Therefore, for $W_{\mathbf{kk}'}$ the Born approximation $W_{\mathbf{kk}'} = V_{\mathbf{kk}'}$ is correct. In the case of large longitudinal dispersion (4), the condition $T \gg \alpha^{-2}$ implies that the Born approximation is correct for all temperatures $T < 1$. When we consider large $k_0 \sim k_B \gg \alpha$, we can use the asymptotic value (18) of $= V_{\mathbf{kk}'}$ for large k, $k' \sim k_0$. For $T \ll T_0$ we obtain the following expression for μ:

$$\mu = \mu_0 \gamma n(T), \quad \gamma = (16\pi)^{-1}(k_0^2/M_0\omega_0)^4 (M_0/m)^2,$$
$$n(T) = e^{\omega_0/T}. \tag{35}$$

From this expression, for the parameter values $\gamma \sim 10$ and for $T \sim \omega_0$, we have $\mu \sim 10\mu_0 \sim 10^3$ cm^2/V-sec. This estimate is somewhat higher than for the case of the contact interaction, and points to the ineffectiveness of this sort of scattering in quasi-one-dimensional conductors.

In the case $k_0 = 0$, for $T \ll T_0$ we can use the expansion of $V_{\mathbf{kk}'}$ for small k, $k' \sim (M_0 T)^{1/2} \ll \alpha$. Since there are no exact expressions for the wave functions $\psi_n(x)$ for the case of polar interactions, there remains an undetermined numerical coefficient of order unity in this asymptotic expansion. Therefore, we can obtain an order-of-magnitude estimate for μ:

$$\gamma \sim (\alpha^2 m/M_0)^4, \quad n(T) = (\omega_0/T)^2 \ln^{-2}(\omega_0/T) e^{\omega_0/T}. \tag{36}$$

From this expression, for $\alpha \sim 10$ and $M_0 \sim 10^2 m$ in the region $T \sim \omega_0$, we obtain for μ the estimate $\mu \sim \mu_0 \sim 10^2$ cm^2/V-sec. In the case $T_0 \ll T < 1$ the estimate for μ turns out to be even simpler: $\gamma \sim \alpha^2 m/M_0$, $n(T) = n_0(T)$ and for $T \sim \omega_0$ we obtain an estimate for μ of the same order of magnitude. In the case of small dispersion the value of μ can be found up to a numerical factor in accuracy:

$$\gamma \sim \alpha^{-1}(\omega_0/\alpha\Delta_\perp)^2 (\alpha^4 m/M^*)^{3/2}, \quad n(T) = (T/\omega_0)^{5/2} e^{\omega_0/T}. \tag{37}$$

Therefore, for $\alpha \sim 10$ and $\Delta_\perp \sim 0.1\omega_0$, we have $\gamma \sim 1$ and for $T \sim \omega_0$ the mobility satisfies $\mu \sim \mu_0 \sim 10^2$ cm^2/V-sec. Thus, estimates of μ for the polarization interaction overestimate the mobility, comparable to the maximum value $\mu \sim 10^2$ cm^2/V-sec in TTF-TCNQ (Ref. 52). We note, however, that in certain cases [see e.g. (37)] the simplest estimates of the mobility coefficient in the expression for μ lead to a decrease in mobility by a factor of one to two orders of magnitude. The values of μ obtained in this way are ~ 1–10 cm^2/V-sec, and agree better with the well-known value of $\mu \sim 1$ cm^2/V-sec in conducting TCNQ salts at room temperature.[52,53] These overestimated values of mobility point to the relative ineffectiveness of electron scattering by polar optical phonons in quasi-one-dimensional organic conductors.

6. POLARON MOBILITY IN THREE-DIMENSIONAL CRYSTALS

As was shown in the previous sections, in one-dimensional conductors the phonon dispersion plays a significant role in calculating the mobility. These effects are also important in three-dimensional crystals in which the magnitude of the optical phonon dispersion is not small.[41] Including it leads to changes in the expression for μ, and simplfies the problem of polaron scattering by phonons. In many cases this allows us to solve the mobility problem completely and find the numerical coefficients, which cannot be done for the case of dispersionless phonon models.[38]

In the papers by Volovik, Mel'nikov, and Edel'shtein[36-38] the effective Hamiltonian (13), (14) was obtained for scattering of polarons by photons. The mobility μ was described by an equation of Fokker-Planck type (16), while the two-phonon scattering amplitude $W_{\mathbf{kk}'}$ for a polaron satisfied the three-dimensional equation (15). The general solution of these equations remains unknown, even when optical-phonon dispersion is taken into account

$$\omega_0(\mathbf{k}) = \omega_0 + (\mathbf{k} - \mathbf{k}_0)^2/M_0.$$

In this section we will calculate μ for the case of large phonon dispersion $M_0 \ll M^* \sim \alpha^4 m$. In the strong-coupling case $\alpha \approx 10$, this condition is usually fulfilled, since[41] $M_0 \sim 10^2 m$. As an exmple we consider the crystal NaCl, in which $\alpha = 8$, $M^* \sim 300m$ (Ref. 20), while the quantity $M_0 \approx 30m$ (Ref. 54). In crystals with the NaCl type of simple cubic lattice, there are optical modes with $k_0 = 0$ and $k_0 \sim k_B$; therefore we investigate both cases.

In the first case, for $T \ll T_0 \sim \alpha^2/M_0$ the thermal phonon momentum $k \sim (M_0 T)^{1/2}$ is small compared to α and to $p \sim (M^* T)^{1/2}$. Therefore the mobility μ is described by the three-dimensional Fokker-Planck equation, while we can expand the quantity $V_{\mathbf{kk}'}$ in the first term of the three-dimensional equation (15) in k, $k' \ll \alpha$

$$V_{\mathbf{kk}'} \approx \frac{C_2}{\alpha^3} \frac{(\mathbf{kk}')}{kk'}, \quad C_2 \sim 1. \tag{38}$$

In addition, we can neglect the small $k' \ll k'' \sim \alpha$ in the denominator of the second term and use the three-dimensional identities (23). As a result, we obtain to lowest order in $T/T_0 \ll 1$ and $T_0 \ll 1$ a solution for $W_{\mathbf{kk}'}$:

$$W_{\mathbf{kk}'} \approx V_{\mathbf{kk}'} \frac{k^2}{M_0} \frac{2Q_{\mathbf{k}}^0}{V_{\mathbf{k}'}}, \tag{39}$$

analogous to formula (24). The equilibrium phonon coordinate $Q_{\mathbf{k}}^0$ is determined by the three-dimensional equations (8). Substituting this expression for $W_{\mathbf{kk}'}$ in Eq. (17), we obtain for μ

$$\mu = \mu_0 \gamma n(T), \quad \gamma = \frac{15\pi^3}{C_2^2}\left(\frac{\alpha^2 m}{M_0}\right)^4, \quad n(T) = \left(\frac{\omega_0}{T}\right)^4 e^{\omega_0/T}. \tag{40}$$

This expression differs[38] from Eq. (2) by the functions $\gamma(\alpha)$ and $n(T)$. We note that in Eq. (40) these functions are grouped into a large factor $(T_0/T)^4 \gg 1$; however, for $\alpha \approx 10$ and $T \sim \omega_0$ this factor turns out to be rather small. We should emphasize that expression (40) is correct for all temperatures $T < T_0$ and does not involve any lower bounds of the type $\alpha^{-2} \ll T \ll 1$ which might restrict the region over which formula (2) is accurate at low temperatures.[38]

In the case $k_0 \sim k_B$ we can use an asymptotic expansion of the type (18) for $V_{\mathbf{kk}'}$ when k, $k' \sim k_0 \gg \alpha$. An estimate of the integral term in the three-dimensional equation (15) shows that it is small when $\alpha^2/M_0 \ll 1$ and $\alpha/k_0 \ll 1$, and therefore for

$$W_{\mathbf{k}\mathbf{k}'} = V_{\mathbf{k}\mathbf{k}'} = 2^{5/2}\pi\alpha k_0^{-4}$$

the Born approximation is correct. The finale expression for μ has the form

$$\gamma = {}^9/_2\pi(k_0^2/M_0\omega_0)^4, \quad n(T) = (\omega_0/T)^2 e^{\omega_0/T}. \tag{41}$$

In this case $k_0^2 \sim M_0\omega_0$ and $\gamma \sim 1$. Thus, the expression for μ (41) differs from Eq. (2) (Ref. 38) only by the temperature-dependent factor $n(T)/n_0(T) = (\omega_0/T)^3$. We note that the smallness of the Born-approximation $W_{\mathbf{kk}'} \sim \alpha k_0^{-4} \ll \alpha^{-3}$ does not imply that $\mu \sim \mu_0$ for $T \sim \omega_0$. This is explained by the fact that inclusion of the integral term in (15) leads to a decrease in the total amplitude $W_{\mathbf{kk}'} \ll V_{\mathbf{kk}'}$, since only by virtue of this smallness can the small denominator in this term be canceled. Hence, the smallness of $W_{\mathbf{kk}'}$ is balanced by the large phase volume in the integral over $\mathbf{k}$, $\mathbf{k}'$ (17), and the non-numerical expression for μ when $T \sim \omega_0$ turns out to be the same as (2), (41). Usually, the case $k_0 \sim k_B$ is more often encountered in ionic crystals,[41] and therefore formula (41) gives the most general expression for μ.

In conclusion, we note that for $\alpha \approx 10$, $m \approx 0.1 m_0$ and $\omega_0 \approx 0.01$ eV, the quantity $\mu \sim \mu_0$ for $T \sim \omega_0$ amounts to 10^2 cm^2/V-sec for all the cases (2), (40), (41) in agreement with the experimental data for alkali-halide compounds.[20]

7. INTERACTION WITH ACOUSTIC PHONONS

The deformation interaction with one-dimensional acoustic phonons[9,10,14–18] is an important mechanism which gives rise to formation of polaron states in quasi-one-dimensional organic conductors and conducting polymers.[6–8] These phonon modes are observed in experiments on the low-temperature lattice heat capacity of $(\mathrm{CH})_x$.[39]

The Hamiltonian for the deformation interaction of an electron with one-dimensional acoustic phonons has the form (3) if we substitute $\mathbf{k} \to k_x$, $\omega_\mathbf{k} = s|k_x|$ and $V_\mathbf{k} = |k_x|(\alpha s^2\omega_1)^{1/2}$ The dimensionless interaction constant α is expressed through the deformation potential D, the mass M_1 of a unit cell and the lattice constant a:

$$\alpha = D^2/2M_1 s^2\omega_1, \quad \omega_1 = 2s/a. \tag{42}$$

Substituting into (42) the typical values $D = 3$ eV, $s = 10^6$ cm/sec, $a = 1.4$ Å, $M_1 = 13$ a.u. for $(\mathrm{CH})_x$,[25] we obtain $\alpha \approx 4$. In the case of PDA,[21] for $D = 3.7$ eV, $s = 3.6 \times 10^5$ cm/sec, $a = 4.9$ Å, $M_1 = 420$ a.u. we have $\alpha \approx 12$.

In order to calculate the acoustic polaron spectrum $\varepsilon(p)$ for any velocity $v < s$, we must transform to a reference frame moving with velocity v in the original Hamiltonian (3). This leads to a Doppler shift in the phonon frequency $\omega_\mathbf{k} \to \tilde{\omega}_\mathbf{k} = \omega_\mathbf{k} - \mathbf{kv}$. The spectrum $\varepsilon(p)$ in such a system for $\alpha \gg 1$ is determined by the classical minimum of the Hamiltonian (3) and in units $\hbar = m = s = 1$ has the form

$$\varepsilon = J + pv,$$

$$J = \frac{1}{2}\int dx \left(\frac{\partial\psi_0}{\partial x}\right)^2 - \frac{1}{2}\sum_{k_x} \frac{V_{k_x}V_{-k_x}}{\tilde{\omega}_{k_x}\tilde{\omega}_{-k_x}} (\psi_0^2)_{k_x}(\psi_0^2)_{-k_x}. \tag{43}$$

Here the momentum $p = M^*v$ is determined by the effective mass M^* given by (9), which because of the Doppler shift depends on v:

$$M^* = \sum_{k_x} \frac{k_x^2 V_{k_x}V_{-k_x}}{(\tilde{\omega}_{k_x}\tilde{\omega}_{-k_x})^2} (\psi_0^2)_{k_x}(\psi_0^2)_{-k_x}. \tag{44}$$

The expressions (43), (44) so obtained determine $\varepsilon(p)$ and agree with the results of using the Lagrangian formalism.[27]

Minimizing the functional J with respect to ψ_0 leads to Eqs. (10), (11), in which it is necessary to include the renormalized interaction constant $\tilde{\alpha} = \alpha/(1 - v^2)$. This leads to the well-known expressions for M^* and J[14]:

$$M^* = 2\alpha^2/3(1 - v^2)^3, \quad J = -\alpha^2/6(1 - v^2)^2. \tag{45}$$

For $v \to 1$ the quantity $pv \sim \alpha^2(1 - v)^{-3}$ is large compared to $J \sim \alpha^2(1 - v)^{-2}$, and therefore the polaron spectrum has a linear character, $\varepsilon(p) \approx p$. The asymptotic expressions for $\varepsilon(p)$ and $v(p) = \partial\varepsilon/\partial p$ have the following forms in this limiting case:

$$\varepsilon(p) \approx p(1 - {}^3/_4(2\alpha^2/3p)^{1/3}), \quad v(p) \approx 1 - {}^1/_2(2\alpha^2/3p)^{1/3}, \quad p \gg \alpha^2. \tag{46}$$

We note that the asymptotic values of $\varepsilon(p)$ and $v(p)$ for $p \gg \alpha^2$ are attained more slowly than for three-dimensional piezopolarons (1).[27]

As follows from Eq. (46), $v(p) \to 1$ as $p \to \infty$, since only for $v < 1$ can the polaron well manage to move together with the electron. For velocities $v > 1$ there is no polaron state, which is obvious from Eq. (43) in which for $v > 1$ the interaction changes sign. In this region a free electron state can exist with energy $p^2/2$ for a given momentum p. This state possesses a much higher energy for a given p than the polaron; moreover, this difference grows rapidly as p increases, since for $p \to \infty$ the polaron energy satisfies $\varepsilon(p) \approx p \ll p^2/2$. Thus, for low phonon bath temperatures $T \ll \alpha^2$, free electrons will rapidly accumulate in the polaron well in a time on the order of an inverse phonon frequency. In the high-temperature case $T \gtrsim \alpha^2$, the polaron states can decay in a thermal fashion; however, because of their large energetic advantages $1/2\,p^2 \sim \varepsilon(p) \gtrsim T$ an electron will be found in the polaron well for an appreciable fraction of the time.

In conclusion we note that because of the strong renormalization $\tilde{\alpha} = \alpha/(1 - v^2)$, the effective interaction constant $\tilde{\alpha}$ can become quite large as $v \to 1$ even for a small bare $\alpha \ll 1$. It is curious that in one-dimensional systems this effect turns out to be much stronger than in three-dimensional systems,[27] where the renormalization has a logarithmic form.

Saturation of the velocity $v(p)$ of an acoustic polaron as $p \to \infty$ leads to a characteristic saturation of the drift velocity v_0 in strong electric fields E. This effect has been observed recently in polydiacetylene PDA[21] and was analyzed in Ref. 55.

8. CONCLUSION

In the present paper we have investigated the mobility μ of polarons in one-dimensional conductors, and have shown that its characteristic value in polymer materials[21,25] agrees with the experimental data.[1–4,21,23,24] Let us note that the quantity $\mu \sim 10^2$ cm^2/V-sec[23,24] is found to be quite large, and in PDA[21] it can reach 10^5 cm^2/V-sec. The corresponding mean free path is found to be quite sizable, and extends from 10^2a in $(CH)_x$ to 10^5a in PDA. In this connection a question arises as to the role of impurities in these systems, since their concentrations in doped $(CH)_x$ can reach a few percent.[1-4] However, it is possible to show that at room temperature the scattering probability by impurities in $(CH)_x$ is small, and does not seem to have any appreciable influence on the polaron mobility.

As is well-known from x-ray data,[1-4] the doping impurities in $(CH)_x$ are located between polymer chains and interact with electrons via Coulomb's law. Therefore, the Born amplitude W_p for backscattering by these charged impurities for a polaron with a thermal momentum $p\approx(M^*T)^{1/2}\sim k_B$ for $M^*\sim10^2m$ and $T\approx300$ °K can be quite small:

$$W_p=\frac{2e^2}{\hat{\varepsilon}_0}\int_0^\infty\frac{dx\cos(2px)}{(x^2+a_1^2)^{1/2}}=\frac{2e^2}{\hat{\varepsilon}_0}K_0(2pa_1)\approx\frac{2e^2}{\hat{\varepsilon}_0}\left(\frac{\pi}{4pa_1}\right)^{1/2}e^{-2pa_1}\quad\text{for}\quad pa_1>1. \qquad (47)$$

The quantity a_1 in (54) is half the spacing between chains $a_\perp=4.4$ Å (Ref. 25), while the quantity p for $T=300$ °K and $M^*=8\alpha^4/15=500m$ ($\alpha\approx6$) works out to be about 0.7×10^8 cm^{-1} for $m\approx0.2m_0$.[25] Therefore, $pa_1\approx1.5$, $K_0(3)\approx0.03$[56] and $W_p\sim10^{-2}e^2\ll e^2$ for $\hat{\varepsilon}_0\sim10$.[1-4] Thus, the inverse mean free path l_i^{-1} relative to scattering by impurities contains a small factor of order 10^{-4} in addition to the small concentration $c_i\sim10^{-2}$. For this reason the quantity l_i is quite large, and does not lead to Mott localization effects,[50] which are suppressed at high temperatures $T\sim100$ °K because of inelastic scattering by phonons. In the case of PDA, the impurity concentration $c_i\sim10^{-5}$ is found to be extremely small,[21] due to the fact that this material polymerizes directly in the solid phase, and its crystals are dintinguished by their exceptionally high quality.[21]

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