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Piezoelectricity and electron mobility in ZnO

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Abstract : Piezoelectric scattering mobility of electrons for the zinc blende structure is found to vary as $T^{-1/2}$ for all range of low temperatures. This signifies a very high conductivity of the sample and a very high velocity of electrons in it at suitably low temperatures. So substances like ZnO have enormous prospect in searching for room temperature super conductivity.

Keywords : Piezoelectricity, dynamical matrix, electron mobility, phonon.

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1. Introduction

Zinc oxide (ZnO) has been found to be vigorously piezoelectric [1,2] with electromechanical coupling constants which considerably exceed that for quartz. Due to piezoelectricity, there will be an electric polarization associated with the acoustical modes of vibration in ZnO. This may lead to periodic electric potential. From the strain associated with each molecule, the electric polarization may be found by using the form of the piezoelectric tensor determined by the crystal symmetry. The electric potential is calculated by using Poisson's equation. The contribution to electronic scattering by this potential has been calculated. Finally, the temperature dependence of the mobility of electrons has been found to be $\mu \propto T^{-1/2}$, where μ = mobility and T = absolute temperature. So at sufficiently low temperature, the mobility and the velocity of electrons will be very high. So substances like ZnO have enormous prospect in searching for room temperature super conductivity.

2. Calculation of the electron mobility

Consider a complex crystal, in general with s different atoms in a unit cell, each having a mass m_k (k = 1,2,...,s). Let us denote the displacement of the k^{th} atom in the n^{th} cell (n = 1, 2,..., N) from its equilibrium position by u_n^k and the orthogonal projections of this displacement by $u_{n\alpha}^k$ ($\alpha = x, y, z$). The potential energy Φ of the principal region of the crystal is a function of all these $u_{n\alpha}^k$. The classical equations of motion of atoms in the harmonic approximation are of the form

$$m_k \ddot{u}_{n\alpha}^k = -\frac{\partial \Phi}{\partial u_{n\alpha}^k} = -\sum_{n'k'\beta} \Phi_{\alpha\beta}\begin{pmatrix} kk' \\ nn' \end{pmatrix} u_{n'\beta}^{k'} . \qquad (1)$$

Its solution in the form of travelling waves is

$$\tilde{u}_{n\alpha}^k = \frac{1}{\sqrt{m_k}} A_\alpha^k(q) e^{i(q.a_n - \omega t)} , \qquad (2)$$

where $\frac{1}{\sqrt{m_k}} A_\alpha^k (\alpha = x, y, z)$ is the projection of the complex amplitude $\frac{1}{\sqrt{m_k}} A^k$, $q = \frac{2\pi}{\lambda}$, λ = wave length and ω = cyclic frequency. Putting eq. (2) in eq. (1) and dividing by $e^{i(q.a_n - \omega t)}$, we get

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$$\omega^2 A_\alpha^k = \sum_{k'\beta} D_{\alpha\beta}^{kk'} A_\beta^{k'}, \tag{3}$$

where the elements of the dynamical matrix of the crystal are

$$D_{\alpha\beta}^{kk'}(q) = \sum_{n'} \frac{1}{\sqrt{m_k m_{k'}}} \Phi_{\alpha\beta}\begin{pmatrix} kk' \\ nn' \end{pmatrix} e^{iq(a'_n - a_n)}, \tag{4}$$

where $\begin{pmatrix} k \\ \alpha \end{pmatrix}$ numbers the rows and $\begin{pmatrix} k' \\ \beta \end{pmatrix}$ numbers the columns in $D_{\alpha\beta}^{kk'}$. Eigen vectors $e_{jjk}(q)$ of the dynamical matrix $D_{\alpha\beta}^{kk'}(q)$ are given by

$$\sum_{k'\beta} D_{\alpha\beta}^{kk'}(q) e_{jk'\beta}(q) = \omega_j^2(q) e_{jk\alpha}(q), \tag{5}$$

where $e_{jk}\propto$ ($\alpha = x, y, z$) are the components of the eigen vector and $\omega_j^2(q)$ is the j^{-th} eigen value of the dynamical matrix. Dynamical matrix is Hermitian. So its eigen values are real and eigen vectors are orthogonal and since they are determined from a homogeneous system, eq. (5), with an arbitrary factor, they can be normalized to unity. Hence,

$$\sum_{\alpha k} e_{jk\alpha} e^*_{j'k\alpha} = \delta_{jj'} \tag{6}$$

and

$$\sum_{j} e_{jk\alpha} e^*_{jk'\beta} = \delta_{kk'}\delta_{\alpha\beta}. \tag{7}$$

Substitution of $-q$ for q changes all the coefficients. So,

$$e_{jk\alpha}(q) = e^*_{jk\alpha}(-q). \tag{8}$$

We introduce complex normal coordinates $a_j(q,t)$ given by

$$u_{n\alpha}^k = \frac{1}{\sqrt{nm_k}} \sum_{q,j} e_{jk\alpha}(q) a_j(q,t) e^{iq\cdot a_n}. \tag{9}$$

Here, it can be shown that

$$a_j(q) = a_j^*(-q). \tag{10}$$

A plane through origin in the q-space separates q and $-q$. Writing eq.(9) in terms of sums of q's taken on each side of the plane, putting $-q$ for q and using eqs. (8) and (10) we have,

$$u_{n\alpha}^k = \frac{1}{\sqrt{Nm_k}} \sum_{qj}' \left[e_{jk\alpha}(q) a_j(q,t) e^{iq\cdot a_n} + c.c. \right]. \tag{11}$$

Prime at the sum means that the summation over q is performed in one-half of a Brillouin zone. Pieozocrystals have no inversion centre. From eq. (11), displacements of the +ve and –ve ions (labels k = 1, 2) in the continuous medium approximation are

$$u_k(r) = \frac{1}{\sqrt{Nm_k}} \sum_{qj}' \left[e_{jk}(q) a_j(q) e^{iq\cdot r} + c.c. \right] \tag{12}$$

Summation over q is over one-half of the Brillouin zone. The polarization vector is

$$P(r) = \frac{e^*}{\Omega_o} \frac{1}{\sqrt{N}} \times \sum_{qj}' \left(\frac{e_{j1}(q)}{\sqrt{m_1}} - \frac{e_{j2}(q)}{\sqrt{m_2}} \right) a_j(q) e^{iq\cdot r} + c.c.. \tag{13}$$

Poisson's equation gives

$$\nabla^2 \Phi = -4\pi\rho = 4\pi \nabla . P(r) = \frac{i4\pi e^*}{\Omega_o} \times \frac{1}{\sqrt{N}} \sum_{q,j}' q \left(\frac{e_{j1}}{\sqrt{m_1}} - \frac{e_{j2}}{\sqrt{m_2}} \right) a_j(q) e^{iq\cdot r} + c.c.. \tag{14}$$

Therefore,

$$\Phi = -i \frac{4\pi e^*}{\Omega_o \sqrt{N}} \sum_{q,j}' (\hat{q}, h_j) a_j(q) e^{iq\cdot r} + c.c. \tag{15}$$

and

$$h_j(q) = \frac{1}{q} \left(\frac{e_{j1}(q)}{\sqrt{m_1}} - \frac{e_{j2}(q)}{\sqrt{m_2}} \right).$$

The perturbation energy corresponding to the potential (15) is $-e\Phi$.

The first term in eq. (15) describes the process of absorption of a photon $h\omega_{qj}$ by the conduction electron. Making use of plane waves for the electron wave functions we obtain

$$k' = k + q. \tag{16}$$

So the complex conjugate in eq. (15) describes the process of emission of a photon by an electron for which

$$k' = k - q. \tag{17}$$

For long wave acoustic phonons, the circular frequency $\omega_{qj} = v_{qj} q$, where v_{qj} is the sound-velocity that depends on the direction of q.

The electron-phonon interaction at all $T>>1$ K is an elastic interaction. In this approximation we obtain an expression for the relaxation time τ. Now electron mobility $\mu = e\tau/m$, where e = charge and m = mass of an electron. In this way, one ultimately finds the mobility [2]

$$\mu = \frac{0.044\rho v^2 h^2 \varepsilon^2}{4\pi^2 e C^2 m^{3/2} (KT)^{1/2}} \tag{18}$$

where ρ = density, v = acoustic velocity for longitudinal waves, h = Planck constant, ε = static dielectric constant, e = charge and m = mass of an electron, C = piezoelectric constant, K = Boltzmann constant and T = absolute temperature.

For Zinc Blende, $\rho v^2 = 1.14 \times 10^{12}$ dynes/cm^2, $\varepsilon = 8.3$, $C = 4.2 \times 10^4$ stat coul/cm^2. For $T = 300$ K, we get $\mu = 2700$ cm^2/volt-sec. From eq. (18) one gets

$$\mu = 3000 \left(\frac{1}{0.07}\right)^{3/2} \left(\frac{300}{T}\right)^{1/2}, \text{ for ZnO.}$$

Therefore for $T = 1$ K, we get, $\mu = 2.8 \times 10^6$ cm^2/volt-sec.

3. Discussion

The expression for mobility suggests that such temperature dependence of mobility and the value of the same at very low temperatures should encourage its study with novel material. At sufficiently low temperature, the mobility and the velocity of electrons will be very high. So substances like ZnO have enormous prospect in searching for room temperature super conductivity.

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