

Asian Resonance

An Approach For Electrical Conduction



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Abstract

Electrical conductivity is the interaction of electron with the lattice by collision processes in which energy and momentum are exchanged. The electrical conductivity of crystals is one of the most important non-equilibrium properties, which shows that how a system relaxes to its equilibrium distribution. An electron is accelerated by the external field between two collision processes. The scattering of electrons gives rise to the electrical resistivity. The theory of electrical conductivity has been investigated with the help of quantum dynamical approach after considering the model Hamiltonian which consists of the state of a real crystal containing phonon system, electron system, localized impurities and interactions thereof. The interaction of electrons with defect induced localized phonon fields with anharmonic forces, which ultimately gives rise, resistance to electronic transport. An electron is scattered out by lattice vibration, the process is similar to which phonon interact. Consequently the potential on electron is disturbed and gives the possibility of scattering. Analysis shows that the electrical conductivity depends on a large number of scattering events and on crystal characteristics and temperatures. Static defects and thermal vibration of lattice are responsible for the scattering of electrons. Present study shows that electrical conductivity directly depends on electron-phonon scattering. Electron phonon scattering is collectively electron-electron scattering, electron-phonon scattering, cubic and quartic phonon electron scattering. The evaluation of electrical conductivity expression shows that it depends on (i) harmonic force fields (ii) localized phonon fields and (iii) Anharmonic forces. In present study it is shown that the experimental variation for electrical conductivity is similar to the theoretical curves.

Keywords : Electron-Phonon Scattering. Localized Phonon Fields.

Thermal Vibrations. Relaxation Time. External Perturbation.

Introduction

The scattering of electrons gives rise to the electrical resistivity. The free electron model of electric transport i.e. free electrons move through the crystal lattice and they are influenced only by the attractive forces of the ions. Under the influence of ions, the electrons move in a potential which varies from point to point, but whose variation is not random, it has a periodicity which is exactly the same as that of ionic lattice. The electrical resistivity of most metals is dominated at room temperature by collisions of the conduction electrons with lattice phonons and at liquid Helium temperature (40°K) by collision with impurity atoms and mechanical imperfection in the lattice ^[1, 2]. Scattering of electron will only occur when the periodicity of the potential is upset. In past a number of compounds have been found which possess electrical conductivity in solid state ^[3, 4]. Inokuchi and Akamatu ^[5] gave a review on electrical conductivity of semi conductors. Due to the weak intermolecular forces the resistivity of organic solids falls off rapidly with rise in temperature. Temperature dependence of electrical conductivity is the most important feature towards the study of electrical conductivity.

At low T lattice imperfections and IMPURITIES are most responsible for the resistivity. At higher T atoms vibrate with much larger amplitude and therefore atomic vibrations contribute dominantly to resistivity at room temperature. The empirical observation of resistivity due to phonon and resistivity due to imperfection can be expressed in the form of Matthiessen's rule. ^[5]

The Bloch T^5 law ^[7] describes the electrical resistivity at low

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temperature. But this law gives some difficulties both experimentally^[8-10] and theoretically^[11-13]. The observation done by Ekin and co-workers^[8,14] for electrical conductivity revealed that the behavior of electrical resistivity is quite complicated and does not exhibit T^{-5} dependence. At low temperature, the resistivity increases in T^2 instead of the usual T^{-5} dependence^[15,16]. T^2 dependence is usually observed in alloys. A general theory of electrical conductivity of alkali metals at low temperature have been presented by Kaveh and Wisner^[17] and reported that phonon drag contribution is important at very low temperature^[18].

This paper deals with the general theory of electrical conductivity. Here we considered a complete Hamiltonian to study the theory of electrical conductivity. This Hamiltonian constitutes (i) Unperturbed phonon Hamiltonian (ii) Harmonic electron Hamiltonian (iii) Defect induced Hamiltonian and (iv) the anharmonic Hamiltonian. A two electron Green's function is obtained strictly on the basis of many particle systems and then applied to the Kubo formalism.

Kubo formalism of Electrical Conductivity

Many experiments in condensed matter physics measure the linear response to an external perturbation. The external perturbation can be generated by putting the sample in a magnetic field, electric field, optical field, temperature gradient or pressure field and measure the magnetization, electric current, light absorption etc. Linear response means that the signal is directly proportional to the intensity of the external perturbation.

The equation for linear responses for the transport in liquids was first derived by Green.^[19,20] Kubo derived the equation for electrical conductivity in solids^[21,22], and so the formulae called Kubo formulae in the condensed matter physics. In electrical conduction, a time – dependent external electric field,

$$E_{\alpha}^{(ext)}(r, t) = E_{\alpha}^{ext} e^{iqr - i\omega t} \quad (1.1)$$

is applied to the solid. In linear response induced current is proportional to the applied electric field

$$J_{\alpha}(r, t) = \sum_{\beta} \sigma'_{\alpha\beta}(q, \omega) E_{\beta}^{ext} e^{iqr - i\omega t} \quad (1.2)$$

The applied external field $E_{\alpha}^{(ext)}$ induces currents which in turn make other electric fields. The summation of all these fields in the total electric field, which is called $E_{\alpha}(r, t)$

The conductivity σ is the one which responds to the actual electric field in the solid;

$$J_{\alpha}(r, t) = \sum_{\beta} \sigma'_{\alpha\beta}(q, \omega) E_{\beta}(r, t) \quad (1.3)$$

Where

$$E_{\beta}(\vec{r}, t) = \sum_{\beta} \sigma'_{\alpha\beta}(q, \omega) E_{\beta}(r, t) \quad (1.4)$$

and

$$\sigma_{\alpha\beta}(\vec{q}, \omega) = \text{Re}(\sigma_{\alpha\beta}) + i \text{Im}(\sigma_{\alpha\beta}) \quad (1.5)$$

equation (1.3) describes the fundamental

microscopic conductivity $\sigma_{\alpha\beta}(\vec{q}, \omega)$.

The equation (1.3) is correct for a homogeneous material; actual solids are not homogeneous, although crystals are in space-time periodic responses.

$$J_{\alpha}(r, t) = \int d^3r' \int_{-\infty}^{+\infty} dt' \sigma'_{\alpha\beta}(r - r'; t - t') E_{\beta}(r', t')$$

(1.6)

If we consider the dc conductivity which is obtained by taking the limit $q \rightarrow 0$ and $\omega \rightarrow 0$ in that order. Then the conductivity is only real. In beginning only a single frequency is perturbing the system were considered and that

$\sigma_{\alpha\beta}(q, \omega)$ is the response to this single frequency. But actually the system is linear and perturbations at different frequencies act independently, so the total current is then the summation of the responses at different frequencies. The Kubo formula for electrical conductivity is,

$$\sigma_{\alpha\beta}(q, \omega) = \frac{1}{\omega} \int_{-\infty}^{+\infty} dt' e^{i\omega(t-t')} \langle \psi | [J_{\alpha}^{+}(q, t'), \hat{J}_{\beta}(q, t')] | \psi \rangle + i \frac{n_o e^2}{m\omega} \delta_{\alpha\beta} \quad (1.7)$$

The electrical conductivity can be defined in terms of current – current correlation functions as [23]

$$\sigma_{\alpha\beta}(\vec{q}, \omega) = \frac{1}{\omega} \int_0^{\infty} dt e^{i\omega t} \langle \psi | [J_{\alpha}^{+}(\vec{q}, t), J_{\alpha}(\vec{q}, 0)] | \psi \rangle$$

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Electron, Electron Green Function

The Green function

$$+ i \frac{n_0 e^2}{m\omega} \delta_{\alpha\beta} \quad (1.8)$$

where n_0 is electric density .

Using the operator formalism [24] the electrical conductivity expression can be rearranged as.

$$\sigma_{\alpha\beta}(\vec{q}, \omega) = (i/\omega) \left[F_{\alpha\beta}(\vec{q}, \omega) + \left(\frac{n_0 e^2}{m} \right) \delta_{\alpha\beta} \right] \quad (1.9)$$

Electron – Phonon anharmonic Hamiltonian

Considering defect induced electron-phonon anharmonic Hamiltonian as –

$$H = H_{op} + H_{oe} + H_{ep} + H_a + H_d \quad (1.10)$$

where, H_{op} is the harmonic phonon Hamiltonian, H_{oe} is the electron Hamiltonian, H_{ep} is the electron-phonon interaction part, H_a is the anharmonic part and H_d contribution due to defects[25,26].

$$H_{Op} = \frac{1}{4} \sum_{q\sigma} \omega_k (A_k^+ A_k + B_k^+ B_k) \quad (1.10a)$$

$$H_{Oe} = \sum_{q\sigma} \epsilon_q (b_{q\sigma}^+ b_q) \quad (1.10b)$$

$$H_{ep} = g \sum_{q\sigma} (b_{Q\sigma}^+ b_{q\sigma} B_k) \quad (1.10c)$$

$$H_a = \sum \sum_{k_1, k_2, \dots, k_s} V_s(k_1, k_2, \dots, k_s) A_{k_1}, A_{k_2} \dots A_{k_s} \quad (1.10d)$$

$$H_d = \sum_{k_1, k_2} [D(k_1, k_2) A_{k_1}, A_{k_2} - C(k_1, k_2) B_{k_1}, B_{k_2}] \quad (1.10e)$$

where

$$A_k = a_k + a_{-k^+} = A_k^+$$

and

$$B_k = a_k - a_{-k^+} = -B_k^+$$

$A_k(a_{-k^+})$ and $b_{q\sigma}(b_{q\sigma}^+)$ are phonon and electron destruction (creation) operators respectively with phonon wave vector $K (=K_j)$ of branch index j and electron wave vector q and spin σ . ϵ_q stands for the electron energy, ϵ_k phonon energy and g stands for the electron-phonon coupling coefficients respectively, $V_s(k_1, k_2, \dots, k_s), C(k_1, k_2)$ and $D(k_1, k_2)$ represents the anharmonic coupling coefficients, mass change and force constant change parameters respectively.[27,28]

$$G_{qq'}^e(t, t') = \langle \langle b_q^+; b_q \rangle \rangle$$

with the help of equation (1.10) using the equation of motion technique of quantum dynamics [29-33], can be evaluated in the form

$$G_{qq'}^e(\omega) = \frac{-\delta_{qq'}}{\pi[\omega + \epsilon_q - P_{ep}(kq, \omega)]} \quad (1.11)$$

where the response function $P_{ep}(kq, \omega)$ can be obtained is the form

$$P_{ep}(kq, \omega) = P_{ep}^{(o)}(kq, \omega) + P_{ep}^d(kq, \omega) + P_{ep}^{3A}(kq, \omega) + P_{ep}^{4A}(kq, \omega) \quad (1.12)$$

The response function can be expressed in terms of real and imaginary parts $\Delta_{ep}(kq, \omega)$ and $\Gamma_{ep}(kq, \omega)$ known as shifts and widths for electron phonon energies respectively as

$$P_{ep}(kq, \omega + i\epsilon) = \Delta_{ep}(kq, \omega) - i\Gamma_{ep}(kq, \omega), \epsilon \rightarrow 0^+ \quad (1.13)$$

Using equation (4.28) in equation (4.21) we get,

$$G_{qq'}^e(\omega + i\epsilon) = -(\delta_{qq'} / \pi) [\omega + \tilde{\epsilon}_q - i\Gamma_{ep}(kq, \omega)]^{-1} \quad (1.14)$$

where

$$\tilde{\epsilon}_q = \epsilon_q - \Delta_{ep}(kq, \omega) \quad (1.15)$$

and

$$\Gamma_{ep}(kq, \omega) = \Gamma_{ep}^{(0)}(kq, \omega) + \Gamma_{ep}^D(kq, \omega) + \Gamma_{ep}^{3A}(kq, \omega) + \Gamma_{ep}^{4A}(kq, \omega) \quad (1.16)$$

The imaginary part of the Green's function $G_{qq'}^e(\omega)$ takes the form

$$\text{Im} G_{qq'}^e(\omega) = -\frac{\delta_{qq'} \Gamma(kq, \omega)}{\pi[(\omega + \tilde{\epsilon}_q)^2 + \Gamma_{ep}^2(kq, \omega)]} \quad (1.17)$$

The Electrical Conductivity

Putting the value of the Green function from equation (1.17) in equation (1.9) we get,

$$\sigma_{\alpha\beta}^{(1)}(\vec{q}, \omega) = \left(\frac{2}{\pi} \right)^2 \sum_{qQ} P_{\alpha}^{Qq}(\vec{q}) P_{\alpha}^{qQ}(\vec{q})$$

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$$\frac{N^2(\omega)\Gamma_{ep}^2(kq, \omega)}{\omega[(\omega + \tilde{\epsilon}_q)^2 + \Gamma_{ep}^2(kq, \omega)]^2} \quad (1.18)$$

After using Breit-Wigner approximation we have

$$\sigma_{\alpha\beta}^{(i)}(\vec{q}, \omega) = \frac{\left(\frac{2}{\pi}\right)^2 \sum_{qQ} P_{\alpha}^{Qq}(\vec{q}) P_{\beta}^{qQ}(\vec{q}) N^2(\tilde{\epsilon}_q)}{\tilde{\epsilon}_q \Gamma_{ep}(kq, \tilde{\epsilon}_q)} \quad (1.19)$$

The width $\Gamma_{ep}(kq, \omega)$ is a measure of the life time of the scattering events (relaxation

time) $\tau_{ep}^{-1}(kq, \omega)$. Referring to equation (1.16) it is evident that

$$\tau_{ep}^{-1}(kq, \omega) = \left[\tau_{ep}^{(0)}(kq, \omega)^{-1} + \tau_{ep}^D(kq, \omega) \right]^{-1} + \left[\tau_{ep}^{3A}(kq, \omega) \right]^{-1} + \left[\tau_{ep}^{4A}(kq, \omega) \right]^{-1} \quad (1.20)$$

if Matheson's rule is followed for these events

then it reveal that (1) $\Gamma_{ep}(kq, \omega)$ inevitable dependence on the electron-phonon coupling coefficient g, i.e. electrical conductivity shows strong dependence on the electron-phonon interactions. This may be understood in following ways :

- (a) Electrons gains energy from localized phonons present around the impurity sites, and
- (b) Electrons gain energy from the anharmonic phonon fields, which certainly change their nature with temperature and frequency.

(ii) the term Ω is present throughout in $\Gamma_{ep}^{(0)}(kq, \omega), \Gamma_{ep}^D(kq, \omega)$ and $\Gamma_{ep}^A(kq, \omega)$

. Let us examine the nature of Ω in more detail. Under a reasonable approximation of first order if we ignore the defect and anharmonic of contributions to Ω and get

$$\Omega = g^2 \left[2 \epsilon_q (\tilde{n}_k + \omega_k \tilde{n}_k) + \omega_k (\epsilon_q \tilde{n}_k + \omega_k n_k) \right] \quad (1.21)$$

Thermal dependence of $\Gamma_k(\omega)$ invariably makes Ω a function of temperature.

Analysis and Conclusion

The interaction of electrons with defect induced localized phonon fields with anharmonic forces, which ultimately gives rise, resistance to electronic transport. An electron is scattered out by lattice vibration, the process is similar to which

phonon interact. Consequently the potential on electron is disturbed and gives the possibility of scattering. The evaluation of electrical conductivity expression shows that it depends on (i) harmonic force fields (ii) localized phonon fields and (iii) Anharmonic forces.

Considering a complete Hamiltonian and the relaxation times approximation reminds the phenomenological model of lattice thermal conductivity given by Callaway.[34] The

dependence of $\sigma_{\alpha\beta}^{(i)}(\vec{q}, \omega)$ on the magnitude of disorders and anharmonicities infers that electrical conductivity is a function of phonon energy, Fermi energy, temperature and defect concentration.

The term $\Gamma_{ep}^{(0)}(kq, \omega)$ gives the contribution to the energy width at electron energy

$$\epsilon = \epsilon_q. \text{The defect term } \Gamma_{ep}^{(D)}(kq, \omega)$$

exhibits the broadening at $\pm \omega_k, \pm \epsilon_q$. The cubic anharmonic term shows broadening of

delta function at $\pm (\omega_{k_1} \pm \omega_{k_2}), \pm \epsilon_q, \pm \epsilon_q$ and the quartic term show that at $\pm (\omega_{k_1} \pm \omega_{k_2} \pm \omega_{k_3}), \pm \epsilon_q, \pm \epsilon_q$. These all terms are temperature dependent.

At low temperature the $\Gamma_{ep}(kq, \omega)$ contributed by $\Gamma_{ep}^{(0)}(kq, \omega)$ and $\Gamma_{ep}^{(D)}(kq, \omega)$, $\Gamma_{ep}^A(kq, \omega)$ has negligible values. The magnitude of $\Gamma_{ep}^{(D)}(kq, \omega)$ largely depends on the defect concentration. At very low temperature,

$$\sigma_{\alpha\beta}^{(i)}(\vec{q}, \omega) = \left(\frac{2}{\pi}\right)^2 \sum_{qQ} \frac{P_{\alpha}^{Qq}(\vec{q}) P_{\beta}^{qQ}(\vec{q}) N^2(\tilde{\epsilon}_q)}{\Gamma_{ep}^{(0)}(kq, \tilde{\epsilon}_q)} \times \left[\frac{1 - \Gamma_{ep}^D(kq, \tilde{\epsilon}_q)}{\Gamma_{ep}^{(0)}(kq, \tilde{\epsilon}_q)} \right] \quad (1.22)$$

At moderate temperatures

$$\sigma_{\alpha\beta}^{(i)}(\vec{q}, \omega) \cong \left(\frac{2}{\pi}\right)^2 \sum_{qQ} P_{\alpha}^{Qq}(\vec{q}) P_{\beta}^{qQ}(\vec{q}) N^2(\tilde{\epsilon}_q) \times \left[\Gamma_{ep}^{(0)}(kq, \tilde{\epsilon}_q) \right]$$

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$$\times \Gamma_{ep}^D(k_q, \epsilon_q)]^{-1} \times \left\{ \frac{1 - \Gamma_{ep}^{3A}(k_q, \epsilon_q)}{\Gamma_{ep}^{(0)}(k_q, \epsilon_q) + \Gamma_{ep}^D(k_q, \epsilon_q)} \right\}$$

(1.23)

At high temperatures,

$$\sigma_{\alpha\beta}^{(1)}(\vec{q}, \omega) \cong \left(\frac{2}{\pi}\right)^2 \sum_{qQ} \frac{P_{\alpha}^{Qq}(\vec{q}) P_{\beta}^{qQ}(\vec{q}) N^2(\tilde{\epsilon}_q)}{[\Gamma_{ep}^{3A}(k_q, \epsilon_q) + \Gamma_{ep}^{4A}(k_q, \epsilon_q)]}$$

$$\times \left\{ 1 - \frac{\Gamma_{ep}^{(0)}(k_q, \tilde{\epsilon}_q) + \Gamma_{ep}^D(k_q, \epsilon_q)}{\Gamma_{ep}^{3A}(k_q, \epsilon_q) + \Gamma_{ep}^{4A}(k_q, \epsilon_q)} \right\}$$

(1.24)

Present study shows that the electrical conductivity is not a function of electron energy but it depends on a large number of factors i.e. Fermi energy, nature of Fermi surface, phonon energy in the form of single frequency or combination band, temperature, defect concentration and electron phonon coupling.

On the basis of above theory we have tried to analyze the electrical resistivity of pure silicon crystal and silicon phosphorous alloy. Silicon is an element of the fourth group of the periodic table. Each silicon atom has four near neighbors with which it forms covalent bonds in tetrahedral configuration. The specific gravity is about 2.4 and the melting point 1420°C, the dielectric constant is about 13. Fig. (A.1) gives the theoretical values compared with experimental points.[35] The initial resistivity at room temperature is about 140 Ω-cm., but at temperature to 700°k the resistivity reduced to 50 Ω-cm., this behaviour continued to higher range of temperature. Higher the temperature lower the resistivity so with increase in temperature the conductivity increases. This is because with increase in temperature the electron gets energy and overcome the resistance offered by the crystal, so the conductivity increases. This change of the electrical resistivity of silicon crystal with temperature indicates a change in the electrically active impurities. The rapid decrease in resistivity with increase in temperature results from the increase in concentration of electrons and holes which arises from thermal excitation of electron.

The electrical conductivity at room temperature depends on the presence of impurities. It is estimated that ideally pure silicon would have a resistivity of about 106 ohm-cm. By adding the impurity atoms the resistivity can be reduced. Elements of third group give p-type conductivity and element of fifth group give n-

type conductivity. The impurity which gives p-type conductivity are called acceptors and those which give n-type conductivity are called donors. A substitution impurity atom from the fifth group has one more valence electron than is required to fill the four valence bonds with neighboring silicon atoms. In its lowest energy state, this extra electron is weakly bound by the extra charge on the nucleus of the impurity atom. A trivalent impurity atom has one less electron than is required to fill the valence bonds.

The extra electron required to fill the valence about the trivalent impurity gives the atom an effective negative charge, so that it becomes in effect a negative ion. In its lowest state, the positive hole will be weakly bound by electro-static field of the negative ion. The ionization energy is likewise of the order of thermal energy. At room temperature the majority of the acceptor impurities will be dissociated into holes and negative ions. Fig. (A.2) gives the theoretical values compared with experimental values [36].

At high temperature the resistivity falls down hence conductivity increases. This is intrinsic region in which there is approximately equal concentration of electrons holes. At lower temperature the resistivity depends on the impurity content, increasing the amount of impurity lower the resistivity. The rapid decrease of resistivity with temperature in the intrinsic range results from the increase in concentration of electrons and holes which arise from thermal excitation of electrons.

At lower temperature impurities contribute to the scattering, so that the mobilities are higher in the pure samples. The impurity centers which give the largest scattering are the donors and acceptors. Scattering by both ionized and neutral centers is large at low temperatures. At lower impurity concentration, electron – electron interaction is important. These interactions drastically reduce conductivity for low concentration. At low temperature the impurities are effective and offers a large resistance but at higher temperature due to the thermal excitation of electrons the electron get energy and overcome consequently the conductivity increases.

In present study the experimental variation for electrical conductivity is similar to the theoretical curves. Above analysis shows that the electrical resistivity depends on scattering of electrons. Static defects and thermal vibration of lattice are responsible for the scattering electrons. Present study shows that electrical conductivity directly depends on electron-phonon scattering. Electron phonon scattering is collectively electron-electron scattering, electron-phonon scattering, cubic and quartric phonon electron scattering and force constant change and electron phonon coupling constants.

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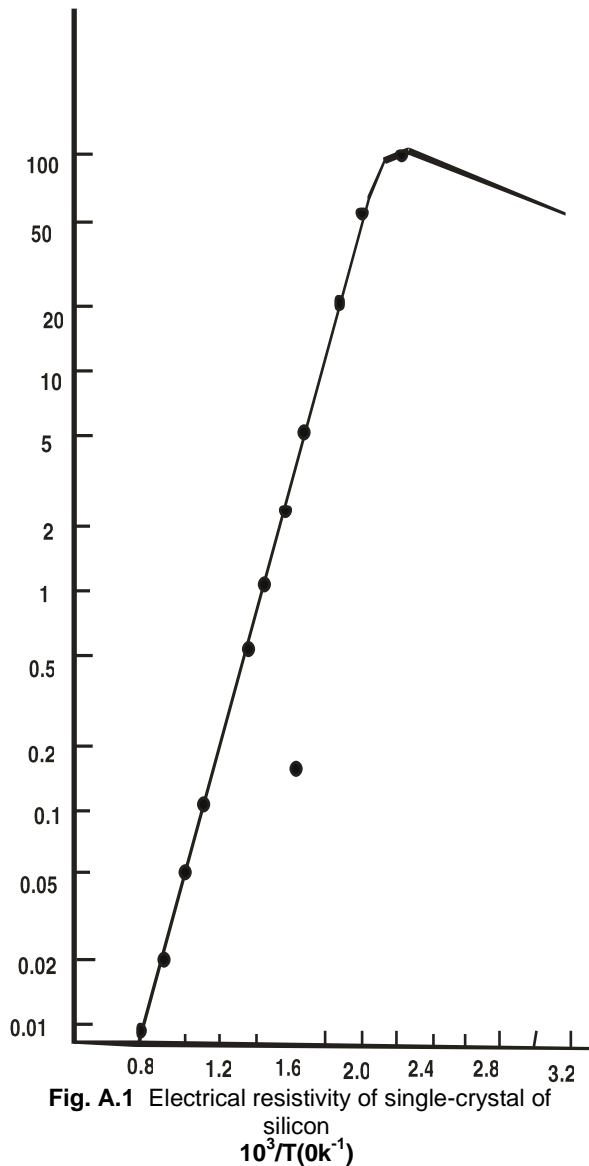


Fig. A.1 Electrical resistivity of single-crystal of silicon
 $10^3/T(K^{-1})$

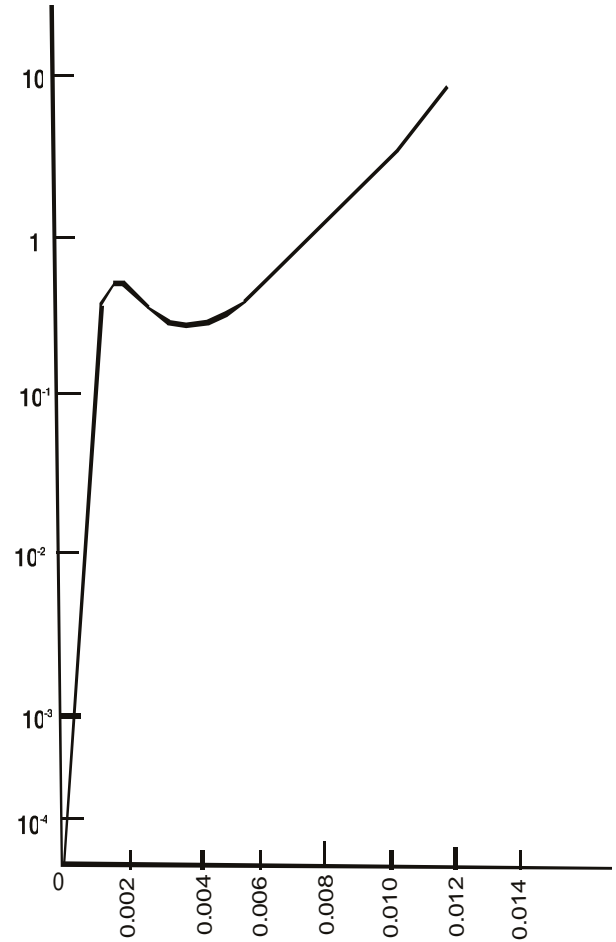


Fig. A.2 Resistivity of silicon –phosphorus alloy
 $[1/Temp]$ in degree Kelvin

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