Theoretical study of some semiconductors under high pressure and high temperature

¹Shankar Singh Rajput, ²Pankaja Singh

¹Research Scholar, ²Professor Department of Physics MVM College Bhopal (M.P.)

Abstract: High pressure research is also a specialized field of physics research in the same manner just as study below 20 K represents a field for low temperature specialists. High pressure physics is a challenging branch of physics, in which one has to produce, apply and measure high pressure on the material and study the physical properties at a given pressure simultaneously. This means that these pressures need to be sustained for times long enough. The pressure dependence of (magnetization per unit mass) of iron and nickel under hydrostatic pressure up to 0.25 k bar and found that the variation is too small to be determined quantitatively. But the author found that $\partial \sigma/\partial p$ was negative for iron and positive for nickel. A subsequent repeat of these measurements by the same workers gave negative values for this pressure effect in nickel also.

Keywords: High pressure, crystal structure, Semiconductor, conductivity and high temperature

1.1 Introduction to Semiconductors

On account of the explosion of information technology and computing, the late twentieth century has come to be regarded as the semiconductor age. The technological impact of these materials will be extremely familiar to the reader, so we consider here the atomic level structure of these materials.

Structurally, most semiconductors consist of a network of covalent bonds leading to an open crystal structure which, like water, becomes denser on melting. They typically exhibit a series of high pressure phase transitions to progressively denser structures and have thus become a paradigm for high pressure studies. The group IV elements and III-V compounds exhibit tetrahedral coordination under ambient conditions, typically in the diamond structure in specific case that has been discussed here, (zincblende or wurtzite in compounds). The application of high-pressure probes the physics of interatomic bonding extremely thoroughly: it gives rise to more dramatic changes in the physical properties of semiconductors than can be attained through temperature variation alone, including bandgap closure and metallization. Metastable the Long-lived structures property of covalent materials to form but, it is not surprising that the high-pressure, combined with the properties of semiconductors are at the forefront of crystallographic parameter.

Chemically, the diamond structure can be regarded as a network of covalent bonds, with secondary ionic bonding giving rise to zinc blende or wurtzite ordering in the III-V compounds. Electronically these semiconductors are semiconducting Application of pressure tends to broaden the electron bands and hence reduce the bandgap: in most cases the first pressure-induced phase transition corresponds to the closing of the bandgap and metallization of the sample: an example of this occurs in tin where the familiar metallic β -tin can be transformed into a grey crumbly powder at low temperature. To conduct the study this has been for the diamond structure i.e. α -tin [1].

A final important effect of pressure in semiconductors, Out with the scope of this review, is its ability to affect the local structure around a crystal defect, and consequently to move the electronic levels associated with such defects. This requires relatively low pressures compared to those involved in phase transitions, and makes pressure a valuable tool for investigating the nature of the defects which give rise to donor or acceptor levels.

1.2 B Group IV Elements

1.2.1 Carbon (C)

Carbon exhibits two unusual features which make it worthy of separate treatment: sp² bonding and extremely high energy of the first d-band. There are four observed crystalline forms of carbon: graphite and fullerene crystals represent low pressure forms based on sp² bonding which otherwise occurs only in BN. Diamond is a high pressure form, while Lonsdaleite (hexagonal diamond) is sometimes found in meteorites or shock-wave recovered samples. Obviously, diamond anvil cells are unable to reach pressures above which diamond transforms, so recent experimental work has left the high pressure phase diagram of diamond untouched. Computationally, it was discovered that 'close-packed' structures are not only energetically unfavoured in carbon, but also have larger equilibrium volumes per atom than the 'open' diamond structures [2]. As a consequence the only high pressure phase transition predicted in early studies was to BC8, at 1100GPa. More recently, ideas for structures have turned to analogues of those observed in other materials, and several structures have been proposed which appear to be more stable than diamond at extremely high pressures.

A productive source of contender structures has come from taking into consideration the positions of the silicon atoms in various phases of SiO₂, which also forms linked tetrahedral networks [3] the oxygen's occupy the positions of 'covalent bonds' in the purported carbon structures). Another possibility is the R8 phase [4], predicted to be more stable than diamond above 910 GPa. By analogy with silicon, this would be kinetically hindered from transforming back to cubic diamond, producing instead hexagonal diamond; consistent perhaps by means of the Lonsdaleite carbon established in samples recovered commencing elevated pressure

[5] confirmed that beneath intense pressure diamond carbon could be melted, [6] have considered melting of BC8 and simple cubic carbon at high pressure and suggested a phase diagram.

Thus it is likely that an as-yet undiscovered phase of carbon exists at pressures above that where diamond is stable. However, the reported energy differences between the competing predicted structures are small, and formation kinetics may play an important role, so the precise structure remains an open question. Although the predicted pressures are high, they are comparable with those at the centres of large planets were carbon is believed to be prevalent.

1.2.2 Silicon (Si)

Silicon exhibit a plethora of constant and metastable high pressure structures which have been exposed since [7] reported the initially in 1962. [8] Since of its position as the archetypal material for high pressure investigation, several group have worked on silicon and the nomenclature of the range of structures has turn out to be confused. The sequence of thermodynamically steady low temperature phases with escalating pressure appeared to be the diamond-*Imma*-SH-*Cmca*-hcp-fcc, where the orthorhombic "Si-VI" phase [9-11] has only recently had its crystal structure identified ([12-13] *Cmca* symmetry and a (16 atom unit cell).

The β -tin phase is experiential at room temperature and pressures flanked by diamond and *Imma* stability, but calculations and theoretical analysis recommend it will not persist to 0 K.

Additional complications take place from the irreversibility of these transitions: formerly silicon has passed from beginning to end its first phase conversion to β -tin the equilateral stage cannot be improved simply by de-pressurization. As a substitute depressurized silicon transforms all the way through two indistinct semimetallic tetrahedral phases which total vigor calculations show to be metastable: R8 and BC8 [14-15], or surface conventional [4]. The BC8 phase persists for the foreseeable future at ambient pressure and room temperature, but on heating transforms to what was in the beginning reported as a hexagonal diamond structure, but now seems more likely to have a more complex or arbitrary stacking sequence as discussed in section IVA. [16] Total energy calculations in silicon have proved remarkably accurate: [17] Needs and Martin (1984) posited that the reported ' β -tin' phase should be unstable with respect to a soft-mode transition to *Imma*, improved experimental resolution made this structure detectable by [18]. The soft approach associated with this and the transition to simple hexagonal, leads to enhanced superconductivity in these phases ([19]. The *Imma* β -tin energy differences are very small [20] predict that *Imma* is stable at all pressures (at 0K) while FP-LMTO 15 calculations by [21] do find a region of β -tin constancy. Since the β -tin phase has higher entropy, both of these calculations can be regarded as dependable with the room temperature experimental data.

The diamond β -tin phase changeover is kinetically very complicated a mechanism of permanent bend in which the diamond structure in uniaxially compacted along (001) is geometrically probable, but total energy calculations showed it to encompass an enormously high energy obstruction. Rapid pressurization tends to bypass the β -tin stage in general, as do computer simulations using invariable pressure ab initio molecular dynamics. [22] The overturn changeover does not occur at all, further demonstrating the absence of a low energy alteration path.

1.2.3. Germanium (Ge)

Germanium has essentially the same phase diagram as silicon, with the diamond phase transforming to β -tin [23] and then to *Imma* [24] at still higher pressure. There is a much larger stability region of α -tin and *Imma* stability compared to silicon, probably due to effects of the 3d core electrons [25] before the Si-like sequence of simple hexagonal, Cmca [26-28] 16 and hcp is resumed. As with silicon, calculations by [20] suggest that the *Imma* phase is more stable than β -tin at 0K and at all pressures. Since these calculations did not include finite temperature effects, it is plausible that β -tin is stabilised only by entropy effects. Like silicon, β -tin phase germanium does not return to diamond on depressurization, forming instead another distorted tetrahedrally coordinated structure, ST12. Calculation shows ST12 to be a metastable phase, but more stable than BC8. However, on fast depressurization the β -tin phase transforms to BC. As with silicon, the BC8 phase can also decomposes to yet another metastable phase: the experimental data for this phase is quite poor, but the most likely candidate seems to be the randomly stacked tetrahedral phase as observed in heated, depressurized Si .[29]

1.2.4. Tin (Sn)

Tin is unusual in that its metal-insulator transition can be induced by temperature change at ambient pressure as well as pressure increase at low temperature. At low temperatures, the low pressure crystal structures are essentially the same as silicon and germanium, diamond (semiconducting) and β -tin (metallic). At higher pressures between 9.5 and 50GPa [30], [9] a tetragonal deformation of the bcc structure (bct) has been reported, above which the bcc structure is adopted. The c/a ratio of bct tin varies from 0.91 to 0.95 with increasing pressure across its stability region, before jumping discontinuously to 1 (bcc). This is consistent with calculations which show that a graph of energy of bct against c/a has a double minimum structure (one minimum being bcc). The effect of phonon entropy in stabilizing the high temperature phase β -tin has been shown theoretically by [31]

1.2.5. Lead (Pb)

While it is a Group IV element, go ahead to showed none of the structural behavior of Si, Ge and Sn. The dissimilarity between lead and the other group IV elements arises commencing the go beyond of the various electronic bands which does not allocate a distinct *sp3* bonding devoid of mixing with other bands. Lead is metallic and put up the shutters packed (fcc) under ambient circumstances, and goes during a series of phase transitions with increasing pressure.

There is no experimental evidence for a bct distortion of the bcc phase, as observed in tin. Calculations of these structures show a similar sequence at 0K [32-33] has carried out ab initio calculations for phonons in all three phases. Using these in the quasi harmonic approximation he was able to determine the temperature dependence of the phase boundaries from first principles.

1.3 Temperature

1.3.1 High Temperature Electronic Substrate Selection Criteria

The electronic revolution is mainly based on Si and is regarded as the first generation of semiconductor in the past century [34]. Enormous progress in Si-based devices is evident in every segment of the industry and society. More than 98% of the current electronic devices are using Si as the substrate [35]. Domination of Si comes from its material properties which are well understood. However, the operating temperature for devices made from this material is not more than 150°C.

Beyond this temperature, Si-based semiconductor devices are incapable of operating efficiently, especially when the high temperature is combined with a high power, high frequency and high radiation environment [36]. This is attributed to its properties in narrow band gap (1.12 eV) and low thermal conductivity [37]. Band gap is a property of semiconductors that determines the amount of energy required for current to flow in the material.

To overcome this problem, a semiconductor with a wider band gap is a better choice to produce devices for high temperature applications. Wide band gap (WBG) semiconductor offers various advantages, namely, higher temperature stability, higher chemical stability, higher thermal conductivity and higher breakdown field. Examples of WBG semiconductors are silicon carbide (SiC), gallium nitride (GaN) and diamond, with their superior electrical properties making them likely candidates to replace Si in the near future for High temperature electronics (THE) applications. Table 1.1 summaries some of the physical and electronic properties of these materials.

Table 1.1 Comparison of some WBG semiconductor properties with Si for HTE	

Property	Si	GaAs		SiC		GaN	Diamond
100	0.000		3-SiC	4H-SiC	6H-SiC		
Bandgap E ₀ (eV)	1.1	1.4	2.40	3.26	3.02	3.4	5.5
Dielectric constant E _i	11.8	12.8	9.72	9.66	9.66	9	5.5
Thermal conductivity, λ	1.5	0.5	3.2	3.7	4.9	1.3	20
(W/cm K)			27.00		State State		
Electron mobility μ_n (cm ² N-s)	1400	8500	800	10000	400	900	2200
Hole mobility, μ_{ρ} (cm ² N-s)	600	400	40	115	101	150	1600
Breakdown voltage (MV/cm	0.3	0.4	1.5	3.2	3.0	5	10
Electronic maximum operating	150	350	700	700	700	>750	10000
temperature (⁰ C)				1			1
Melting point (K)	1690	1510	3100	3100	3100	2070	>2500
Physical stability	Good	Fair	Excellent	Excellent	Excellent	Good	Very Good
						All of	
Process maturity	Very	High	Medium	Medium	Medium	Very low	Very low
	High	-			The same of the sa	CL 3	

Among the candidates, SiC has emerged as a very shows potential candidate to substitute Si in particular applications, especially in HTE devices. A large quantity of consideration has been given to SiC, which is measured as the a large amount established WBG semiconductor. Due to the large band gap of SiC compare to Si, the earlier enable HTE devices to function powerfully at temperatures beyond 600°C [35]. SiC has a number of advantages compare to other WBG materials, as well as the commercial accessibility of substrates, known device processing technique, and the capacity to produce thermal oxides. SiC has established large values of the following; band gap: enabling lesser leakage current from temperature induced essential conduction; breakdown electric field: sustaining an eight-fold larger voltage gradient, enabling thinner energetic regions, lower resistance and higher voltage operation; thermal conductivity: at the bottom of four-fold higher power densities than GaAs or Si; saturated electrons drift velocity, twice that of silicon, appropriate for more rapidly operating speeds; bond energy (between Si and C), giving high mechanical strength, chemical inertness, and energy resistance.

An approximately unlimited number of SiC poly types are potential and approximately 200 poly types previously have been exposed. These poly types are differentiate by the stacking sequence of the bi-atomic congested packed layers. The majority of common poly types are hexagonal 6H-SiC and 4H-SiC, cubic 3C-SiC and rhombohedral 15R-SiC. On the other hand, not poly types are easy to produce. Only 4H and 6H poly types are accessible as substrate material could be promoted for application part of semiconducting materials [35].

GaAs is the subsequently a large amount commonly used for semiconductor after Si. Its bandgap is 1.4 (eV), which makes it a appropriate candidate for HTE application. However, Due to the physical properties and difficulties in device fabrication using this material however, it is not extensively used for HTE application [38].

Along with the WBG semiconductor, diamond has the universally superior properties, not matched by any other materials. Obviously, diamond is the material of selection for a lot of applications particularly individuals which require a high operating temperature [35]. Diamond melts at approximately 3827°C. It is constant at eminent temperatures, but its constancy depends on the ambient. But, diamond is regarded as one of the most difficult semiconductors to make a functional device.

1.3.2 Temperature Effects in Semiconductors

In the present study, we discussed the problem of temperature variation at the device and circuit level. In Section 1.1, we provide surroundings on the material dependences on temperature. In Section 1.2, the standard and reverse temperature dependence regimes

are described earlier. In Section 1.3, we examined how these dependences vary with technology scaling and the introduction of new processing materials, such as high-k dielectrics and metal gates.

1.3.3 Material Temperature Dependences

In this section we provide the details about the impact of temperature on the MOSFET energy band gap, carrier density, mobility, carrier diffusion, velocity saturation, current density, threshold voltage, leakage current, interconnect resistance, and electromigration.

1.4 Energy Band Gap

Temperature affects the properties of electronic systems in a number of fundamental ways. The most fundamental of properties is the energy band gap, Eg, which is affected by temperature according to the Varshni's equation [39]

$$E_g(T) = E_g(0) - \frac{\alpha_E T^2}{T + \beta_E}$$
 (1.1)

where Eg(0) is the band gap energy at absolute zero on the Kelvin scale in the particular material, and α_E and β_E are material-specific constants. Table 1.1[40] provides these constants for three material structures. Table 1.1 and (equation 1.1) are used to produce Fig. 1.1, which shows how the band gaps of the three materials decrease as temperature increases (the labeled points are the band gap of each material at room temperature).

Table 2.1 Varshni's equation constants for GaAs, Si, and Ge [40]

Material	Eg (0) (eV)	α _E (eV/K)	$\beta_{E}(K)$
GaAs	1.519	5.41*10 ⁻⁴	204
Si	1.170	4.73*10-4	636
Ge	0.7437	4.77*10 ⁻⁴	235

1.4.1 Carrier Density

Carrier densities affect electrical and thermal conductivity, and are a function of the effective density of states in the appropriate band (conduction for n-type, valence for p-type), the Fermi energy level in the material (which is a function of temperature and dopant concentrations), and the temperature as given by the following equations:

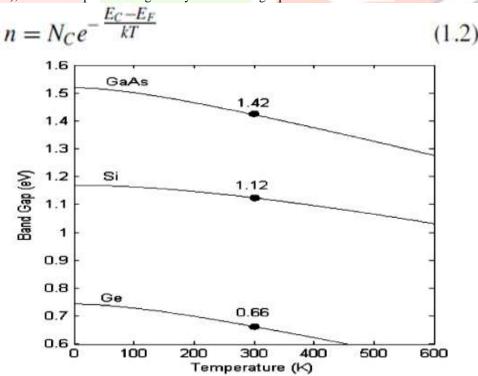


Fig. 1.2 Energy band gap temperature dependence of GaAs, Si, and Ge

$$p = N_V e^{-\frac{E_F - E_V}{kT}} \tag{1.3}$$

where n is the electron density, p is the hole density, NC is the density of states in the conduction band, NV is the density of states in the valence band, EC is the conduction band energy level, EV is the valence band energy level, EF is the Fermi energy level, k \(^{1}\)4 1.38x10^{23} J/K is the Boltzmann constant, and T is temperature. The temperature dependence of carrier density is shown in Fig. 1.2 for a doped material. In the ionization region, there is only enough latent energy in the material to push a few of the dopant carriers into the conduction band. In the extrinsic region, which is the desired region of operation, the carrier concentration is flat over a wide range of temperatures; in this region, all of the dopant carriers have been energized into the conduction band (i.e. n ND) and there is very little thermal generation of additional carriers. As the temperature increases, the extrinsic region turns into the intrinsic region, and the number of thermally generated carriers exceeds the number of donor carriers. The intrinsic carrier concentration in a material ni is generally much smaller than the dopant carrier concentration at room temperature, but ni (\(^{1}\)4n·p) has a very strong temperature dependence [40].

$$n_i \propto T^{1.5} e^{-\frac{E_{g0}}{2kT}}$$
 (1.4)

Where Eg_0 is the energy band gap at T $\frac{1}{4}$ 0 K. depending upon the dopant concentration, the number of thermally generated carriers can exceed the number of dopant-generated carriers, increasing the potential for thermal variation problems.

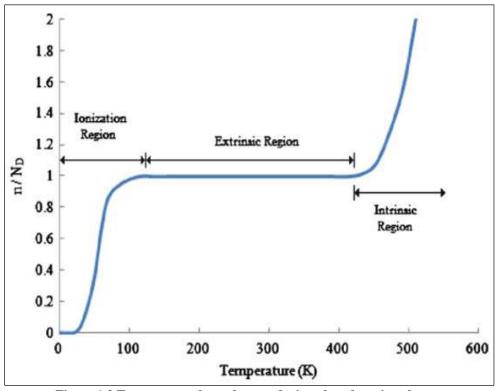


Figure 1.2 Temperature dependences of n in a doped semiconductor

1.4. 2 Carrier Diffusion

Diffusion is the movement of particles from a region of high concentration to a region of low concentration. Carrier diffusion coefficients Dn and Dp (for electrons and holes, respectively) are related to mobility by the Einstein relationship

$$\frac{D}{\mu} = \frac{kT}{q} \tag{1.5}$$

Here, q is the charge on an electron (1.6X 10^{-19} C), and kT/q is an important value known as the thermal voltage, fT. At room temperature (300 K), fT $\frac{1}{4}$ 0.0259 V. Dn and Dp in room temperature silicon are 36 and 12 cm^{2/s}, respectively.

1.4.3 Current Density

The temperature dependence of the carrier concentrations, mobilities and diffusion coefficients affect the temperature behavior of the carrier current densities, with the carrier densities defined by the following formulas [41]

$$J_N = q\mu_n n\xi + qD_n \nabla n \tag{1.6}$$

$$J_P = q\mu_p p \xi - q D_p \nabla p \tag{1.7}$$

Where, JN and JP are the electron and hole current densities, respectively. The first term in each equation is the drift component of the total current, with mn and mp corresponding to the electron and hole mobilities, respectively; x is the electric field. The second term in each equation is the diffusion component of the total current, with ∇n and ∇p corresponding to the electron and hole concentration gradients (if there is no concentration gradient, there is no diffusion). The temperature dependent parameter in the second term is the diffusion coefficient. Increased temperature increases particle kinetic energy, increasing the diffusion component of total current. The drift component of the total current has two temperature dependent parameters, the mobility and the carrier density. The mobility decrease as temperature increases (in the lattice vibration-limited case) while the carrier density remains nearly fixed with temperature over the extrinsic range (our intended range of operation), as indicated by Fig. 1.2. Thus, we determine that the drift component of the total current decreases as temperature increases.

The drift and diffusion currents have opposing temperature dependencies, which causes the net current change to depend on the applied electric field. In the high-field (drift-dominated) case, current decreases as temperature increases; in the low-field (diffusion-dominated) case, current increases as temperature increases. However, if the system in question is a multi-voltage system, and the system has both drift- and diffusion-dominated components, the impact of temperature variation may become less well-defined. The difference between a drift dominated system and a diffusion-dominated system is defined by the threshold voltage, VT. We will show that the temperature dependences of mobility and threshold voltage result in some very interesting device behavior. [41]

1.4.4 Leakage Current

Subthreshold leakage current Isub is exponentially dependent on temperature, a common rule of thumb is that leakage current doubles for every 10^{-C} increase in temperature [42]. When, VGS ¼ 0, Isub may be represented by the Shockley diode model.

$$I_{sub} = I_0 \left(e^{\frac{V_{DS}}{\phi_T}} - 1 \right) \tag{1.8}$$

1.5 Temperature Dependence of Semiconductor Conductivity (resistivity)

1.5.1 Theory Band Structure of a Semiconductor

The band structure of semiconductors is such that the outermost band of electrons, the valence band, is completely full. If a voltage is applied, there is no conduction of electrons because there are no empty spaces to allow the electrons to move around. In order for conduction to occur, electrons must be excited to the next highest band, known as the conduction band. The conduction band is normally empty but is separated from the valence band by only a small amount of energy. Valence electrons can surmount this barrier by absorbing a small amount of energy from heat or light. This then creates a free electron in the conduction band and a hole (missing electron) in the valence band, Callister.

Doping (replacing Si atoms with atoms of another element) is frequently used instead of temperature to control conductivity. Doping can be localized to certain areas whereas the affect of temperature is a less localized influence. If Si is replaced by elements from Column V of the periodic table such as phosphorous, there will be one extra electron in the valence band, Callister. This electron is easily broken loose to create a free electron. Silicon doped with Column V elements in known as p-type and the dopants are called donors. Replacing Si with an element from Column III (such as boron) creates a hole in the valence band. The silicon is known as n-type and the dopants are called acceptors.

1.5.2 Conductivity of a Semiconductor

The conductivity of a semiconductor is given by:

$$\sigma = q(\mu_n n + \mu_p p) \tag{1.9}$$

Where, µn and µp refer to the mobilities of the electrons and holes, and n and p refer to the density of electrons and holes, respectively. A *doped* semiconductor, majority carriers greatly outnumber minority carriers, so that Equation 1.9 can be reduced to a single term involving the majority carrier.

1.5.3 Effects of Temperature and Doping on Mobility of a Semiconductor

Conductivity of a material is determined by two factors: the concentration of free carriers available to conduct current and their mobility (or freedom to move). In a semiconductor, both mobility and carrier concentration are temperature dependent. Thus, it is important to view the conductivity as a function of temperature which is expressed by:

$$\sigma = q \left[\mu_n(T) n(T) + \mu_p(T) p(T) \right] \tag{1.10}$$

There are two basic types of scattering mechanisms that influence the mobility of electrons and holes: lattice scattering and impurity scattering. We have already discussed lattice scattering in the context of metals; we know that lattice vibrations cause the mobility to decrease with increasing temperature.

However, the mobility of the carriers in a semiconductor is also influenced by the presence of *charged impurities*. Impurity scattering is caused by crystal defects such as ionized impurities. At lower temperatures, carriers move more slowly, so there is more time for them to interact with charged impurities. As a result, as the temperature decreases, impurity scattering *increases* and the mobility *decreases*. This is just the opposite of the effect of lattice scattering.

The total mobility then is the sum of the lattice-scattering mobility and the impurity-scattering mobility. Figure 1.3 shows how the total mobility has a temperature at which it is a maximum. The approximate temperature dependence of mobility due to lattice

scattering is $T^{-3/2}$, while the temperature dependence of mobility due to impurity scattering is $T^{+3/2}$ (Fig. 1.3). In practice, impurity scattering is typically only seen at very low temperatures. In the temperature range we will measure, only the influence of lattice scattering will be expected.

1.5.4 Temperature Dependence of Carrier Concentration

The carrier concentration in a semiconductor is also affected by temperature. The intrinsic carrier concentration is governed by:

$$n_i(T) = 2 \left[\frac{2\pi kT}{h^2} \right]^{\frac{3}{2}} \left(m_n^* m_p^* \right)^{\frac{3}{4}} \exp \left[\frac{-E_g}{2kT} \right]$$
 (1.11)

Where, the exponential temperature dependence dominates ni (T). To determine the total carrier concentration, we must also consider space-charge neutrality:

$$n(T) = N_D^+(T) - N_A^- + \frac{n_i^2(T)}{n(T)} \qquad \text{and:} \qquad p(T) = N_A^-(T) - N_D^+(T) + \frac{n_i^2(T)}{p(T)}$$
 (1.12)

For a doped semiconductor, the temperature dependence of electron concentration can be seen in Figure 1.4 at very low temperatures (large 1/T), negligible intrinsic electron-hole-pairs (EHPs) exist (ni is very small), and the donor electrons are bound to the donor atoms. This is known as the *ionization* (or *freeze-out*) region. As the temperature is raised, increased ionization occurs and at about 100 K all of the donor atoms are ionized, at which point the carrier concentration is determined by doping. The region where every available dopant has been ionized is called the *extrinsic* (or *saturation*) region. In this region, an increase in temperature produces no increase in carrier concentration. Referring to Equation 1.12, this is the region where, N_D^+ (T) = N_D , N_A^- (T)= N_A , and $n_i(T) < |N_D^- N_A|$. At high temperatures, the thermally generated intrinsic carriers outnumber the dopants ($n_i > |N_D^- N_A|$). In this *intrinsic* region, carrier concentration increases with temperature as shown in Equation 3 because n_i has become the dominant term of Equation 1.12.

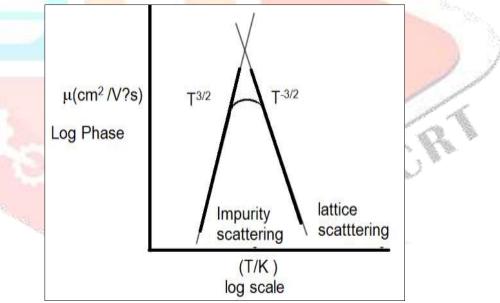


Figure 1.3 Approximate temperature dependence of mobility with both lattice and impurity scattering

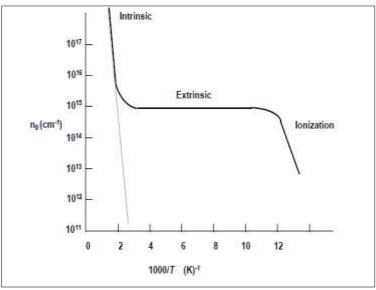


Figure 1.4. Carrier concentration vs. reciprocal temperature for silicon doped with 10¹⁵ donors/cm3

1.5.5 Temperature Dependence of Conductivity for a Semiconductor

Remember that Equation 1.9 showed that conductivity depends on both carrier concentration and mobility, so there are a variety of possible temperature dependencies for conductivity. For instance instance, at fairly low temperatures (less than 200K), the dominant scattering mechanism might be impurity scattering ($\mu \alpha T^{3/2}$) while the carrier concentration is determined by extrinsic doping ($n = N_D^+$), therefore, conductivity would be seen to increase with temperature ($\sigma \alpha T^{3/2}$). Other possibilities, depending on the material, doping, and temperature will show different temperature dependence of conductivity. One particularly interesting case occurs at high temperatures (above 400K or higher) when carrier concentration is intrinsic (Equation 1.12) and mobility is dominated by lattice scattering ($\mu \alpha T^{3/2}$). In such cases, the conductivity can easily be shown to vary with temperature as: [43]

$$\sigma \propto \exp\left(\frac{-E_g}{2kT}\right)$$
 (1.13)

In this case, conductivity depends only on the semiconductor bandgap and the temperature. In this temperature range, measured conductivity data can be used to determine the semiconductor bandgap energy.

1.6 Conclusion

In this study the effect of hydrostatic and quasi hydrostatic pressure on the electrical and optical properties of semiconductors. The presently available pressure range for truly hydrostatic pressures such as developed in shear-free fluids is 30 kilobars. Higher pressures, up to 500 kilobars, may be obtained quasi-hydrostatically by immersing a sample in a soft matrix of silver chloride or some other easily sheared substance to which force can be a applied while the material is constrained in volume. Our particular concern will be to evaluate the extent to which such research has contributed to our present knowledge of semiconductor properties, to examine whether and how further research should be carried out, and to discuss the contribution of a program of research at the extremely high pressure now available. We shall not discuss non-hydrostatic effects such as those caused by uniaxial tension, although these are very useful in studying semiconductor crystals of high symmetry; nor shall we discuss the properties of those substances which are semiconducting only at pressures or temperatures substantially higher than in our normal environment.

References

- [1] Ackland, G.J., 1991, Phys.Rev.B. 44, 3900; 1989 Phys.Rev.B. 40, 10351
- [2] Fahy S., and Louie S.G., 1987, Phys. Rev. B, 36 3373.
- [3] Teter, D.M., Hemley, RJ, Kresse, G. and Hafner, J. 1998, Phys. Rev. Letters 80, 2145
- [4] Clark,SJ, Ackland,GJ and Crain,J. 1995 Phys.Rev.B 52, 15035
- [5] Galli, G, Martin, RM, Car, R, Parrinello, M 1990, Science, 250 1547
- [6] Grumbach, M.P. and Martin, R.M. 1996, Phys. Rev. B 54, 15730.
- [7] Minomura, S and Drickamer, H.G. 1962, J.Phys. Chem. Solids 23, 451.
- [8] Ruoff, A. L., and Li, T. 1995 Annual Rev. Mat. Science 25, 249.
- [9] Olijnyk, H. and Holzapfel, W.B. 1984 J. de Physique, 45, 153.
- [10] Duclos, S.J, Vohra, Y.K. and Ruoff, A.L. 1990, Phys. Rev. B., 41, 12021.
- [11] Vijaykumar, V and Sikka, S.K. 1990, High Pressure Research 4 306.
- [12] Hanfland,M, Schwarz,U, Syassen,K, Takemura,K Phys Rev Letters, 1999, 82, 1197

- [13] Ahuja, R, Eriksson, O, Johansson, B 1999 Phys. Rev. B. 60, 14475
- [14] Crain, J., Ackland, GJ, Maclean, J.R., Piltz, R.O. Hatton, P.D. and Pawley, G.S. 1994, Phys.
- [15] Pfrommer, BG, Cote, M, Louie, SG, Cohen, ML Phys. Rev B, 1997, 56, 6662
- [16] Besson, JM, Mokhtari, EH, Gonzales, J and Weill, G, 1987 Phys. Rev. Lett 59 473.
- [17] Needs R. J., and Martin, R.M. 1984, Phys. Rev. B. 30, 5390.
- [18] McMahon M. I., R. J. Nelmes, N. G. Wright, D. R. Allan, 1994, Phys. Rev. B. 50, 739.
- [19] Mignot, J.M., Chouteau, G. and Martinez, G 1986, Phys. Rev. B 34 3150.
- [20] Lewis, SP and Cohen, ML 1994 Solid State Comm 89, 483
- [21] Christensen, N.E., 1998, Semiconductors and semimetals, 54 49.
- [22] Bernasconi, M., Chiarotti, G.L., Focher, P. Scandolo, S. Tosatti, E. and Parrinello, M. 1995, J. Phys. Chem. Solids 56, 501.
- [23] Baublitz, M., and Ruoff, A.L., 1982, J. Appl. Phys. 53, 6179.
- [24] Nelmes, RJ, McMahon, MI Phys. Rev. Lett, 1996, 77, 663
- [25] Vohra, Y. K, Brister, KE Desgreniers, S. Ruoff, AL Chang, KJ and Cohen, ML, 1986, Phys. Rev. Lett. 56, 1944.
- [26] Ribeiro, FJF and Cohen, ML 2000 *Phys. Rev. B* 62 11388.
- [27] Takemura, K., Schwarz, U., Syassen, K., Christensen, N.E., Hanfland, M. and Novikov, D.L. 2001 *Phys. Stat. Solidi B* 223, 385.
- [28] Mujica, A, Radescu, S, Munoz, A. and Needs, RJ Phys. Stat. Solidi B, 2001, 223 379.
- [29] Nelmes, RJ, McMahon, MI, Hatton, PD, Crain, J, Piltz, RO Phys. Rev. B, 1993, 48, 9949
- [30] Barnett, J.E., Bean, V.E. and Hall, H.T. J. Appl. Phys 37 875 (1966)
- [31] Pavone, P. Baroni, S, de Gironcoli, S Phys. Rev B., 1998, 57, 10421.
- [32] Liu, A.Y., Garcia, A., Cohen, M.L. Godwal, B.K. and Jeanloz, R. 1991 Phys. Rev. B. 43, 1795.
- [33] Swift,D. 1999, PhD thesis, University of Edinburgh.
- [34] McCluskey, F.P., Grzybowski, R. and Podlesak, T. (1997). CRC Press, p.322.
- [35] M. Willander, Friesel, M., Wahab, Q. and Straumal, B. (2006). *Material in Electronic 17: 1-25*.
- [36] Casady, J.B. and Johnson, R.W. (1996). *Solid-State Electronics* 39: 1409-1422.
- [37] Werner, M.R. and Fahrner, W.R. (2001) Industrial Electronics, IEEE Transactions on 48: 249-257.
- [38] Dreike, P.L., M.Fleetwood, D., King, D.B., Sprauer, D.C. and Zipperian, T.E. (1994) Components, Packaging, and Manufacturing Technology, Part A, IEEE Transactions on 17: 594-609.
- [39] Varshni YP (1967) Temperature dependence of the energy gap in semiconductors. Physica 34:149–154
- [40] Sze SM (1981) Physics of semiconductor devices, 2nd ed. John Wiley and Sons, NY
- [41] Pierret RF (1988) Semiconductor fundamentals, 2nd ed. Addison-Wesley, MA
- [42] Oxner ES (1988) FET technology and application. CRC Press, NY
- [43] Callister, Materials Science and Engineering: An Introduction, Chapter 19.6-19.12
- P.W Bridgman, Compressibilities and Electrical Resistance Under Pressure, with Special Reference toIntermetallic Compounds, *Proc. Am. Acad. Arts Sci.*, *Volume 70*, *pp.285-317*, *1935*
- [45] H. Kamerlingh Onnes, Akad. van Wetenschappen, Amsterdam 14, 113, 818 (1911).
- [46] W. Paul and D.M. Warschauer, MC Graw-Hill Book Company, Inc. NewYork (1963).
- [47] H. Nagaoka and K. Honda, Phil. Mag. Series 5 46, 261 (1898).