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FUNDAMENTALS OF METAL-SEMICONDUCTOR CONTACTS

by

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The metal-semiconductor (m-s) contact is one of the oldest semiconductor devices [1], yet even today it is not completely understood. Schottky [2] originally described the basic device, shown in Fig. 1. It is merely a metal in direct physical contact with a semiconductor with the barrier height determined by bulk metal and semiconductor properties. The fact that real devices do not behave in this simple manner (Fig. 2), is attributed to surface states at the semiconductor surface [3]. The mechanism by which this comes about is shown in Figs. 3 and 4.

Bardeen [3] assumed that there were intrinsic surface states at the semiconductor surface prior to metal deposition and that these, if present in a sufficient density, could pin the surface Fermi level to some energy making the barrier height relatively independent of the metal work function. It has been shown [4] that for many semiconductors, the barrier height is approximately 2/3 of the bandgap for n-type and 1/3 of the bandgap for p-type materials.

The nature of the surface states is not well understood. The termination of the bulk lattice at the surface will introduce dangling bonds, the surface morphology being different from that in the bulk and various impurities on the surface are some of the mechanisms giving rise to surface states [5].

The deposition of the metal alters the nature of these surface states. Recent work by Spicer [6] suggests that in the metal deposition process, defect levels are created in the semiconductor. For a sufficiently high defect density, the surface Fermi level should be pinned to the defect energy level. This is shown in Fig. 5 for GaAs. The location of the Fermi level coincides with the EL2 antisite defect energy levels. This defect is the result of an As atom occupying a Ga site, and it has been suggested [7] that such antisite defects are created at the surface by the deposition process.

Because the exact details of surface states and their role in m-s contacts are not well understood, it is clear that "m-s engineering", i.e. designing the barrier height to a specific value, can in general not be done. The closest to such a realization are silicide-silicon contacts [8] in which the interface is located below the original silicon surface because silicon is consumed in the silicide formation process. This appears to reduce or eliminate surface state related effects. The resulting nearly

linear proportionality between barrier heights and work functions is shown in Fig. 2. For metals, however, it is virtually impossible to make ohmic contacts of the "accumulation" type, although such contacts are preferred because of their low barrier heights. A good example is shown in Fig. 6 for Al/n-Si [9]. The Schottky argument would predict a barrier height of 0.2V, while in reality it is observed to be 0.6-0.7V.

This raises the question "how do we make good ohmic contacts?" The energy band diagrams of a m-s contact with increasing semiconductor doping and constant barrier height are shown in Fig. 7. As the doping concentration is increased, it becomes progressively easier for electrons to tunnel from the metal to the semiconductor and from the semiconductor to the metal, because tunnelling depends chiefly on the width of the barrier. The higher the tunnelling probability the lower the contact resistivity. This is clearly shown in Fig. 6. An additional factor that helps to reduce the contact resistivity is barrier lowering [10], shown in Fig. 8.

An ohmic contact is characterized by a contact resistance, related to the contact resistivity in a complicated manner as a result of the current flow. The front contact of a solar cell is as shown in Fig. 9. The current flows through the thin n-surface layer into the contact causing current crowding at the edge of the contact. To first order, the voltage in the diffused layer under the contact decays exponentially with a characteristic transfer length, L_T . It depends on both the contact resistivity, ρ_c , and the sheet resistance, R_s , and is a measure of that part of the contact that is active in the current flow from the diffused layer to the metal. Once the current is in the metal, it of course spreads out due to its low resistivity.

The expression for the contact resistance is given in Fig. 10. It incorporates both geometrical factors as well as ρ_c and R_s [12,13]. Fig. 11 indicates that for typical sheet resistances of 30-100 ohms/square, typical of solar cells, L_T can be very short. For $\rho_c = 10^{-4}$ ohm-cm², it is only 10 μ m, so that even if the contact is 100 μ m wide, only 10 μ m around the edge participates in the transfer of current from the diffused layer to the metal. The normalized plot of Fig. 12 shows the contact resistance multiplied by the length of the contact as a function of the contact width, L. It clearly shows that when L exceeds L_T , the contact resistance is constant and making the contact wider does not result in lower contact resistance. Widening the contact will, however, reduce the grid line resistance but will also increase shading of the cell.

What contact resistance values are required for solar cells? The series resistance of solar cells is the sum of several components, as shown in Fig. 13. Clearly all of these must be optimized, but here we are only concerned with the front and back contact resistance. A first order calculation in Fig. 14 assumes (i) the power loss due to series resistance is 5% [14], and (ii) the contact resistance contributes 10% of the total resistance, i.e. 0.5% of the power loss. The calculated contact resistivities are 10^{-3} ohm-cm² for conventional one-sun applications and 10^{-5} ohm-cm²

for concentrator 100-sun applications. The requirements for the back contacts are less severe because the contact area is equal to the cell area. This is shown in Fig. 15.

Experimentally determined contact resistivities for Si [15, 16, 17] and GaAs [18] are shown in Figs. 16 and 17. Values for p-Si are less than those for n-Si, because the barrier heights are lower. Limiting values of around 10^{-8} ohm-cm² are approached in both cases. The required values of 10^{-5} - 10^{-3} ohm-cm² for n-Si are consistent with typical solar cell surface concentrations of $1-2 \times 10^{20}$ cm⁻³. Most of the data points in Fig. 16 are for Al contacts that are well sintered for optimum resistance. Such low values may be difficult to achieve with plated and silk-screened contacts unless special attention is paid to ensure good, intimate contact between the metal and the semiconductor. Low contact resistance and high open circuit voltage places two conflicting requirements on the doping concentration of the n-layer, as shown in Fig. 18. In practice, the "higher" requirement has usually been chosen.

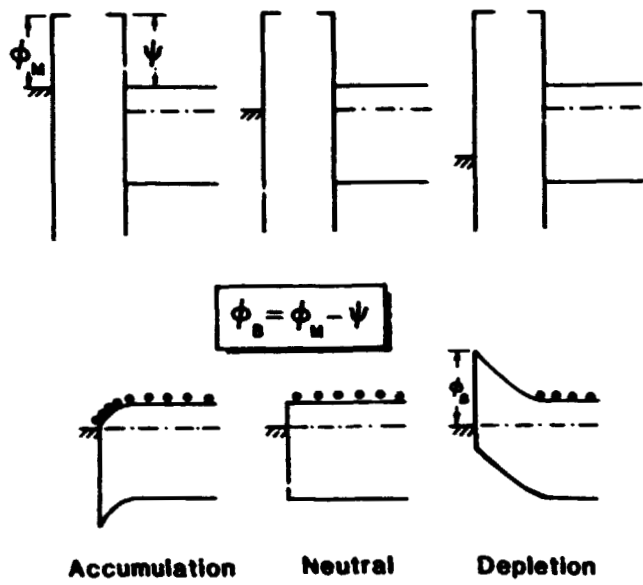
The discussion so far has dealt with a m-s contact that is "ideal" in the sense that there is uniform, intimate contact between the two, even though surface states are present. The surface state problem is overcome by using a heavily doped semiconductor. A "real" contact, however, is not this simple. It may look like that in Fig. 19. Generally there is a layer of oxide or other contaminant between the two with the result that the metal makes random contacts to the semiconductor and alloys non-uniformly [19]. In addition penetration of metal into the diffused layer causes spiking or even penetration of layers of only 0.1 μ m thickness. For example, Al/Si often shows a high degree of non-uniformity, generally along the periphery of the contact, which can be eliminated by adding a small amount of Si or Cu to the Al [19]. The contaminant layer may be of little significance if it is sufficiently thin that tunnelling can proceed freely. If it is too thick, then the contact resistance will increase sharply.

It is clear that with proper surface preparation very low resistance contacts can be achieved. For low-cost solar cells, where cost-effective contacting methods like plating and silk-screening are being pursued, care must be exercised to ensure the low resistance contacts required for the cell's performance. This is especially true for concentrator applications where the photocurrent increases and $I^2 R_s$ losses can become serious.

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Figure 1. Schottky Model



$$J = A^{**} T^2 \exp(-q\phi_b/kT) (\exp(qV/kT) - 1)$$

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Figure 2. Barrier Heights

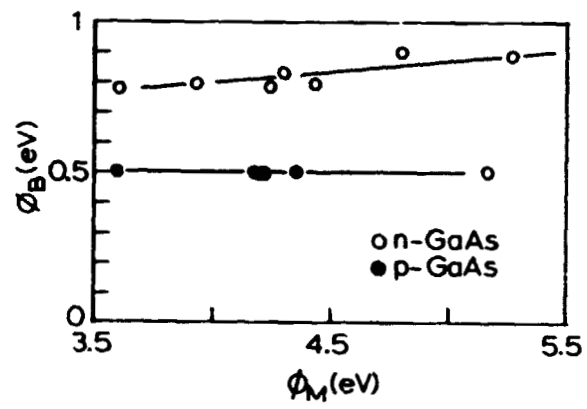
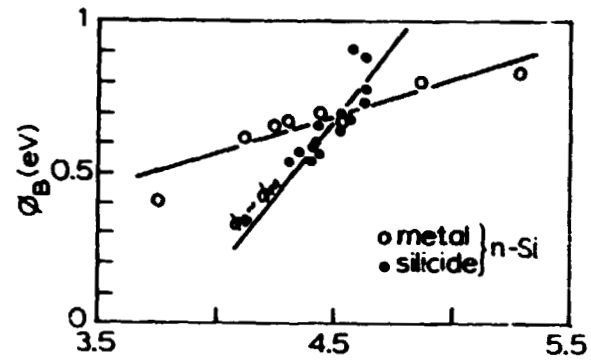
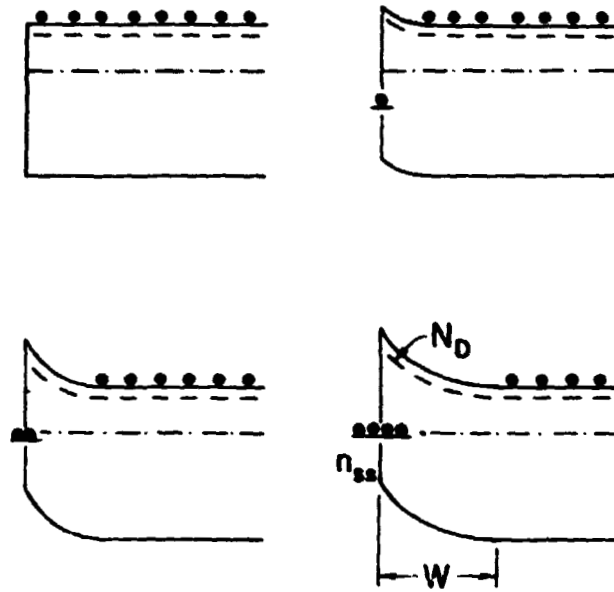


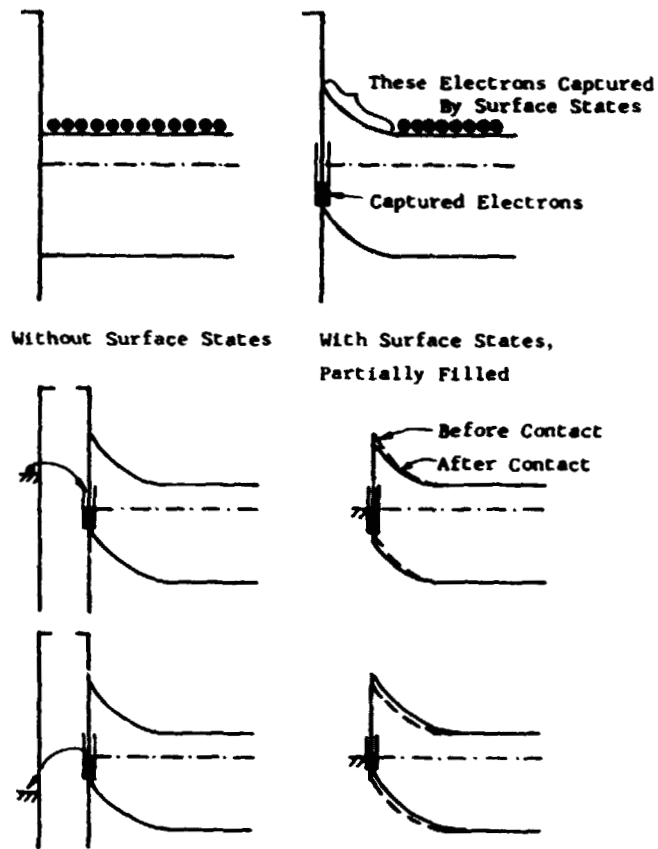
Figure 3. Effect of Surface States

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$$n_{ss} = N_D W$$

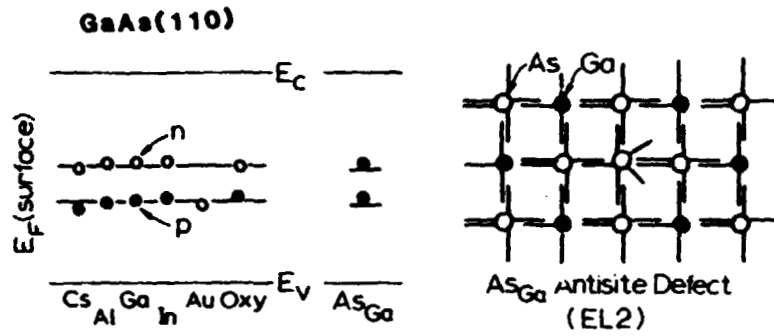
Figure 4. Bardeen Model



$$\phi_s = S(\phi_M - \psi) + C$$

Figure 5. Spicer Model

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- E_f pinning independent of atom
- E_f pinning completed by less than one monolayer of atoms
- Adsorbed atoms disturb surface, creating defect levels

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Figure 6. Example: Al-n-Si

$$\phi_M(\text{Al})=4.25 \text{ V}; \psi(\text{Si})=4.05 \text{ V}$$

Hence should get $\phi_B=0.2 \text{ V}$; in reality $\phi_B=0.6-0.7 \text{ V}$

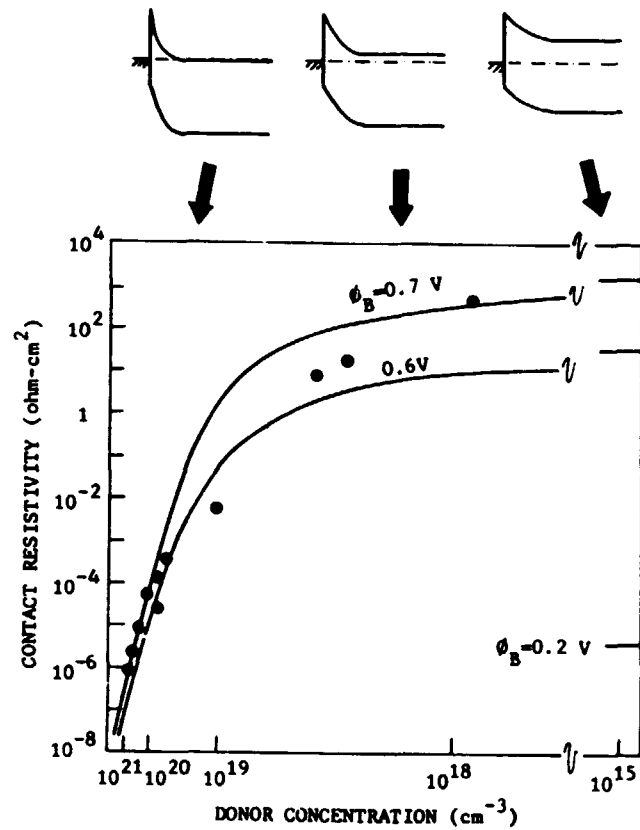
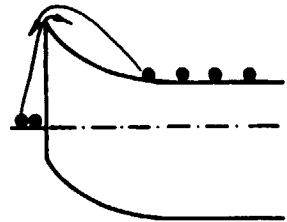


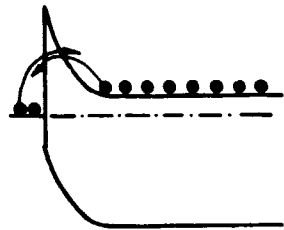
Figure 7. Barrier Width-Doping Concentration



$$P_c \sim e^{q\phi_b/kT}$$

$$\sim 10^8 \Omega \text{ cm}^2 \text{ for } \phi_b = 0.7 \text{ eV}$$

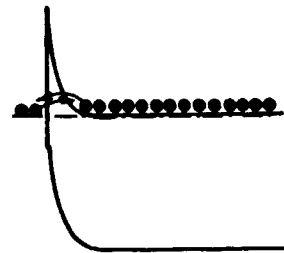
Low N_D -Thermionic Emission



$$P_c \sim 1/N_D$$

$$\sim 1-100 \Omega \text{ cm}^2$$

Intermediate N_D -Thermionic/Field Emission

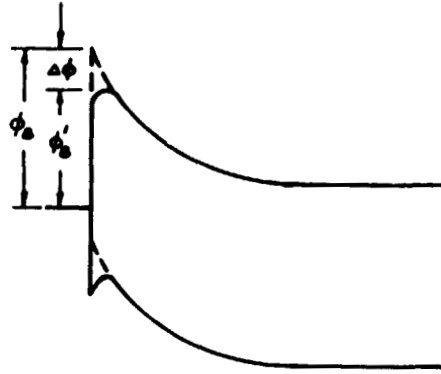


$$P_c \sim e^{\kappa\phi_b/\sqrt{N_D}}$$

$$\sim 10^{-8} - 10^{-2} \Omega \text{ cm}^2$$

High N_D -Field Emission

Figure 8. Barrier Lowering



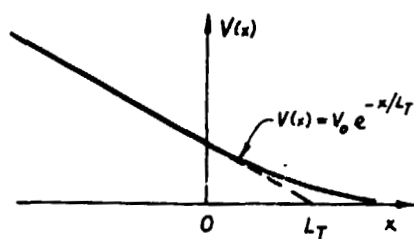
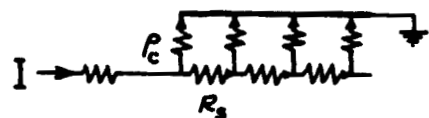
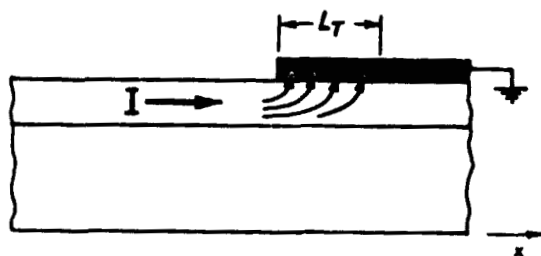
$$\Delta\phi = \left(\frac{qE}{4\pi k_s \epsilon_0} \right)^{1/2}$$

$$E = \frac{qN_D W}{k_s \epsilon_0} \quad W = \left(\frac{2k_s \epsilon_0 \phi_0}{qN_D} \right)^{1/2}$$

for Si:

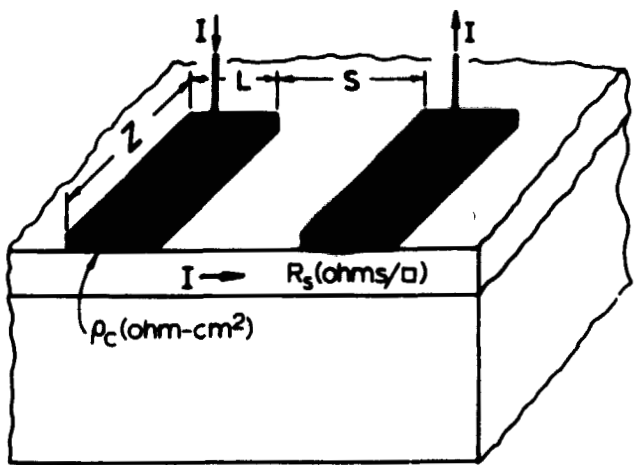
N_D (cm^{-3})	10^{18}	10^{17}	10^{20}
$\Delta\phi$ (eV)	0.08	0.13	0.24

Figure 9. Contact Current Crowding



$$L_T = \sqrt{\rho_c / R_s} \quad (\text{Transfer Length})$$

Figure 10. Layer and Contact Resistance

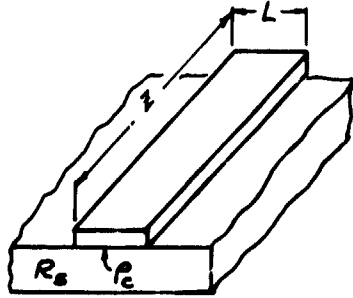


$$R = R_s(S/Z) + (2 L_T/Z) R_s \coth(L/L_T)$$

$R_{\text{layer}} \qquad R_{\text{contact}}$

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Figure 11. Transfer Length, Contact Resistance

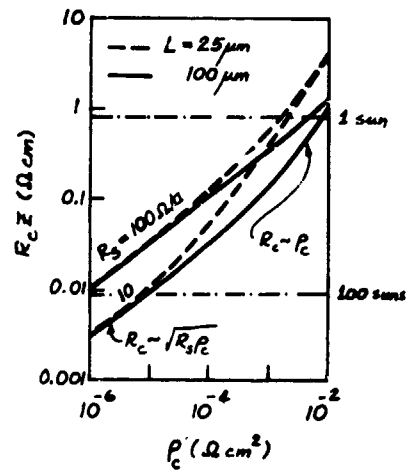
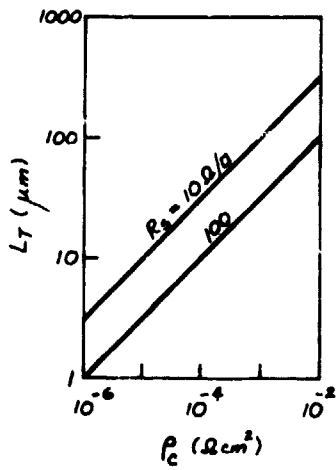


$$L_T = \sqrt{\rho_c / R_s}$$

$$R_c = (L_T / z) R_s \coth(L / L_T)$$

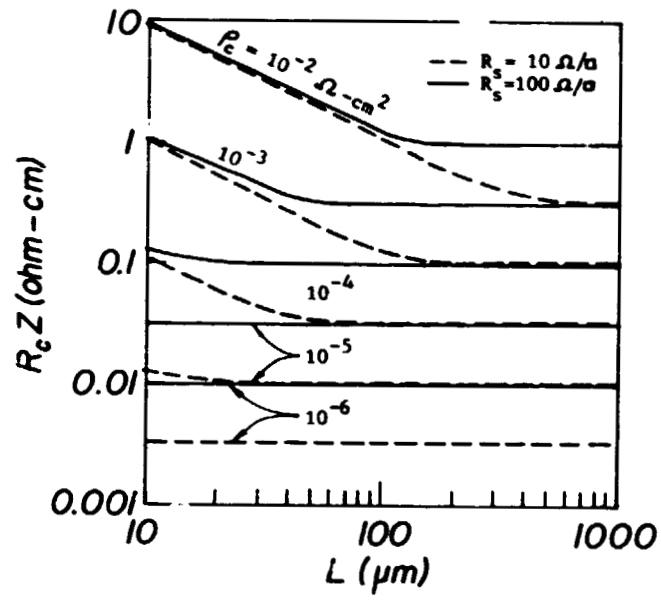
$$R_c \approx L_T R_s / z \quad \text{for } L \geq 1.5 L_T$$

$$R_c \approx \rho_c / L z \quad \text{for } L \leq 0.5 L_T$$



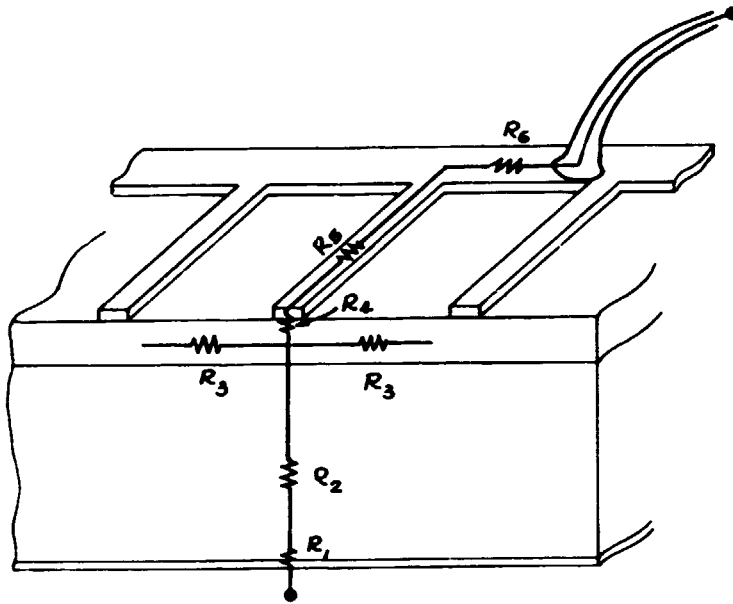
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Figure 12. Contact Resistance, Contact Size



C-2

Figure 13. Solar-Cell Series Resistance



$$R_s = \sum_{i=1}^6 R_i$$

- | | |
|------------------------|-----------------------|
| R_1 = back contact | R_4 = front contact |
| R_2 = bulk | R_5 = grid lines |
| R_3 = diffused layer | R_6 = bus lines |

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Figure 14. Front Contact

• Case 1

$$A = 100 \text{ cm}^2 \quad J = 30 \text{ mA/cm}^2 \quad V = 0.5 \text{ V} \quad (\underline{1 \text{ sun}})$$

$$\Rightarrow \underline{P = 1.5 \text{ W}}$$

$$\text{Loss due to } R_s : 5\%, \text{ i.e. } 7.5 \times 10^{-2} \text{ W} = I^2 R_s$$

$$R_s \leq 0.3 \times 10^{-3} \Omega$$

$$\text{Let } R_c(\text{front contact}) \approx 0.1 R_s = 0.3 \times 10^{-4} \Omega$$

$$\text{Let } A(\text{front contact}) \approx 0.05 A = 5 \text{ cm}^2 \\ = 50 \mu\text{m} \cdot z \Rightarrow z = 10^3 \text{ cm}$$

$$\therefore \underline{R_c z \leq 0.83 \Omega \text{ cm}}$$

$$R_c z \approx 0.83 \Omega \text{ cm} \quad L = 50 \mu\text{m} \quad R_s = 100 \Omega/\square$$

$$\Rightarrow \boxed{P_c \leq 10^{-3} \Omega \text{ cm}^2}$$

• Case 2

$$A = 10 \text{ cm}^2 \quad J = 3 \text{ A/cm}^2 \quad V = 0.5 \text{ V} \quad (\underline{\sim 100 \text{ suns}})$$

same arguments

$$\Rightarrow \boxed{P_c \leq 10^{-5} \Omega \text{ cm}^2}$$

Figure 15. Back Contact

• Case 1

$$A = 100 \text{ cm}^2 \quad J = 30 \text{ mA/cm}^2 \quad V = 0.5 \text{ V} \quad (\underline{1 \text{ sun}})$$

$$P = 1.5 \text{ W}$$

for similar loss due to R_s as for front contact

$$R_c \text{ (back contact)} \leq 8.3 \times 10^{-4} \Omega$$

but $A \text{ (back contact)} = 100 \text{ cm}^2$

$$P_c = R_c A$$

$$\Rightarrow \boxed{P_c \lesssim 10^{-1} \Omega \text{ cm}^2}$$

• Case 2

$$A = 10 \text{ cm}^2 \quad J = 3 \text{ A/cm}^2 \quad V = 0.5 \text{ V} \quad (\underline{\sim 100 \text{ suns}})$$

$$\Rightarrow \boxed{P_c \lesssim 10^{-3} \Omega \text{ cm}^2}$$

Figure 16. Contact Resistivity: Si

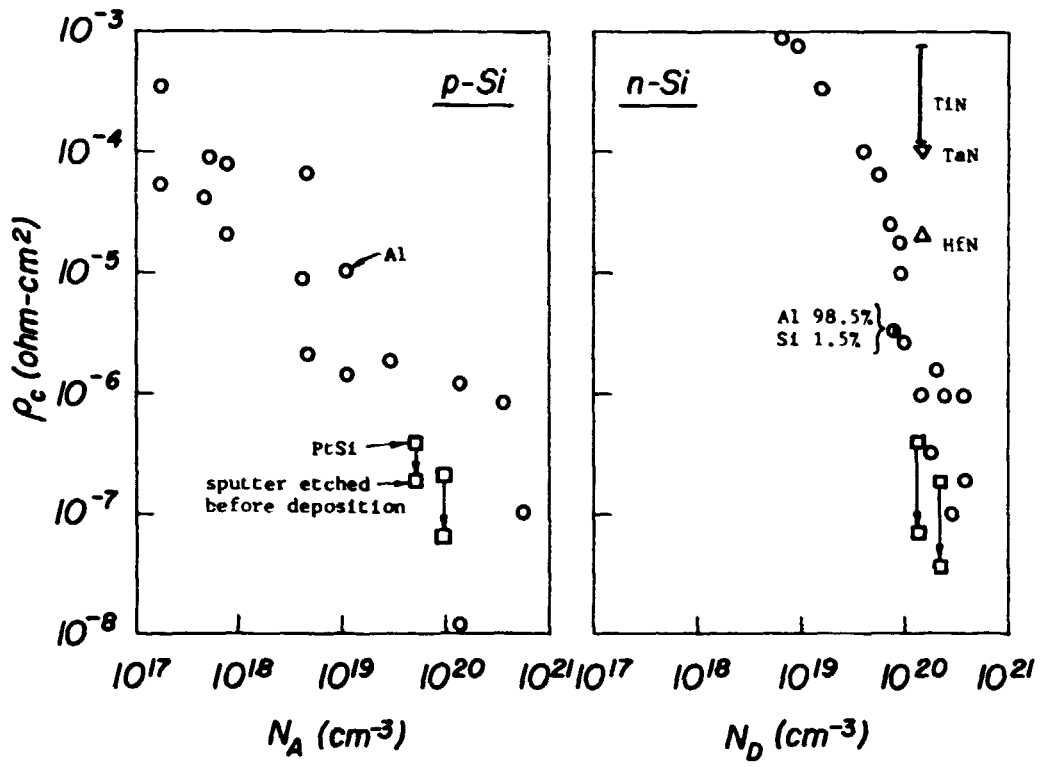


Figure 17. Contact Resistivity: GaAs

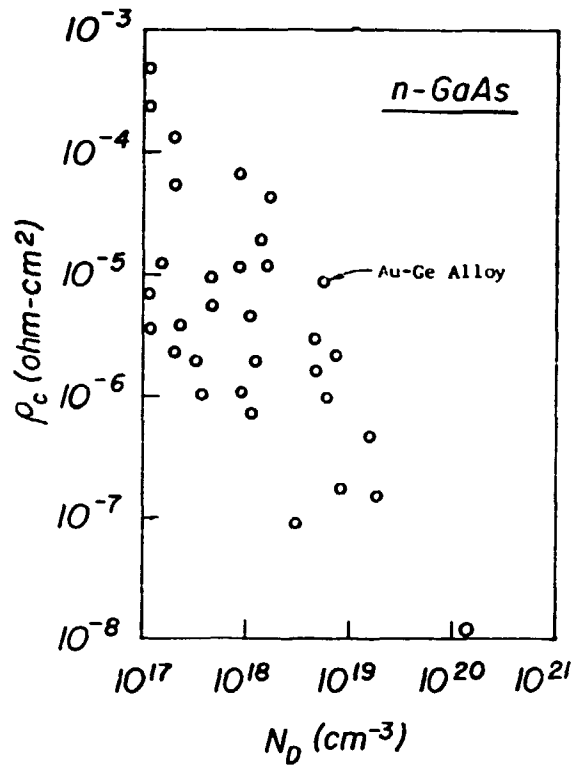


Figure 18. Diffused Layer N_D

• Should be low, because of

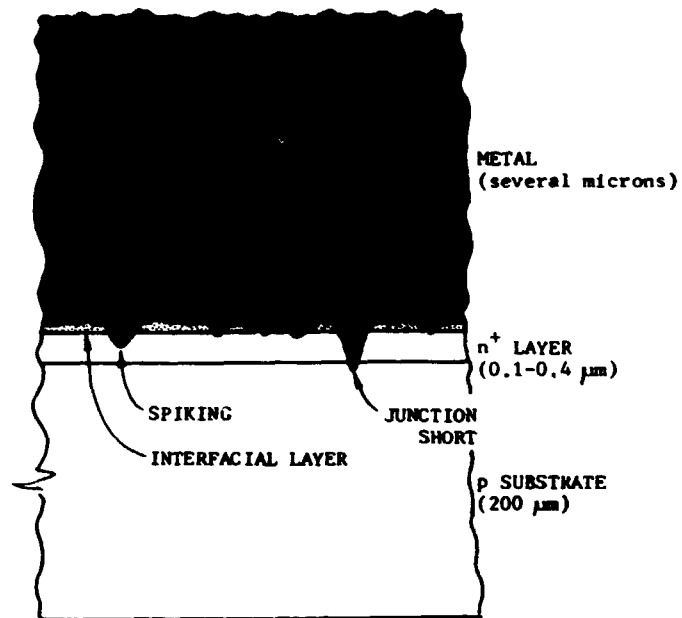
- Bandgap narrowing
- Auger recombination
- Increased Isat
- $N_D \lesssim 1-2 \times 10^{19} \text{ cm}^{-3}$

• Should be high, because of

- Layer sheet resistance
- Contact resistance
- $N_D \gtrsim 10^{20} \text{ cm}^{-3}$

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Figure 19. "Real" Metal-Semiconductor Contact



- Contact area can be much smaller than metal area
- Interfacial layer must be thin for efficient tunnelling ($\leq 25 \text{ \AA}$)

DISCUSSION

HOGAN: Would you comment on the process of annealing, and what might be happening considering gallium arsenide also?

SCHRODER: I think you will see when you read papers and they plot contact resistance as a function of temperature treatment (annealing, for example) that things tend to get better most of the time. Now what goes on? I don't know. Maybe there is an interdiffusion. There can be interdiffusion of metallic species at room temperature. People have found metallic impurities in the semiconductor by not heating it at all, so there is interdiffusion. People are doing a lot of work right now on silicides. I really don't know what the answer is. I don't know what goes on in the contact and I am not sure if anyone else really knows how much interdiffusion really takes place. Does it dope, does it not dope, etc.; we can play all sorts of games, as we heard earlier. If we implant donors or acceptors we can lower or raise the barrier height, and so on, but I think as a rule we don't really understand, not very well anyway.

NICOLET: Would you project the viewgraph with the contact resistivity values? I can give you an upgraded number for titanium nitride.

SCHRODER: This was from a paper two years ago.

NICOLET: We have done Ti-nitride on n as well as on p up about where you have hafnium nitride. About half way; it is 3 or 4 x 10⁻⁵ and it is the same for n and p. That value is 2 after you anneal by 400° or so. If you don't have it before, it is worth noting that in n on p there is a shift in the value height that has to do with certain states, which goes away by annealing and that, we think, comes because we use RF sputtering. If we did that with dc it probably would be less. We have better numbers. It's still high on the rest of these things, but it is more where hafnium nitride is.

SCHRODER: But you don't really need these values for conventional solar cells. I think if you are here you are fine.

NICOLET: Well, up to 30 times concentration of these values --

SCHRODER: Right, exactly. I think if you can do 10⁻⁴, 10⁻⁵, reproducibly, there is no problem. I think it is only when you start moving up to here that you are going to run into problems.

QUESTION: Excuse me, is that using transmission line?

NICOLET: This problem -- this will be published in Solid State Electronics -- the difficulty with making good measurements on these layers is that you have to include the sheet resistivity to the metal layer also. You have to take a double transmission line model -- we can do that in the beginning, learn quite a lot from difficulties -- so we got numbers that attributed voltage difference to the contact resistance while it was due

to the metal. So if you cover that with additional metal to get rid of this or you apply models that include the effect, you get the same result. This is why we are fairly confident that these numbers now are real, honest-to-God numbers for the measurements we have made.

SCHRODER: The measurements are not trivial for these contact resistivities. There was a paper recently that dealt with polysilicon to silicon in which certainly the resistance of the poly becomes very important, and you ought to take that into account, just like you said for the metal, which we normally think of as infinitely conducting. It really isn't.

WOLF: Since you essentially make the entire surface degenerate to make a good ohmic contact -- there was an old method used some decades ago, of mechanically damaging the surface heavily to make a good ohmic contact. Is that a somewhat related method, to essentially make the surface degenerate too?

SCHRODER: I thought about that a little bit and I think what is happening is you have created an enormous number of recombination centers. Normally an ohmic contact is a region of infinite recombinations. That is how we define it from a device viewpoint. So if you, in truth, introduce an enormous number of recombination centers by mechanically damaging the surface, I am not sure I would rely on the reliability of the ohmic contact.