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Germanium-Gallium Arsenide Heterojunctions*

Abrupt monocrystalline junctions between two different semiconductor materials (heterojunctions)[1] have been made by depositing germanium epitaxially on gallium arsenide substrates. The purpose of this communication is to summarize some tentative results obtained in a study of the electrical characteristics of these junctions. A more detailed paper is under preparation.

Germanium can be transported from a hot to a cooler portion of a furnace by a process involving iodine compounds.[2] This method was used here to deposit Ge epitaxially on GaAs. Because of the similarity in crystal structure and lattice constant (5.62 A for both materials) it was expected that there would be negligible strain at the interface. Such strains would tend to complicate interpretation of the measured properties.

The furnace used for this deposition is depicted in Fig. 2 of the Marinace communication.[3] The hydrogen carries the iodine past the germanium, where germanium iodides are formed. The iodides dissociate in the cooler substrate region on the right side of the diagram.

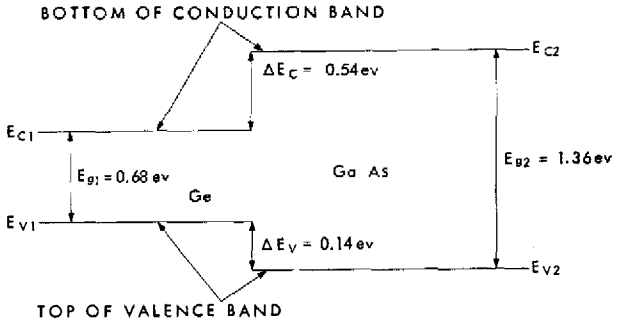
The heterojunctions described here were obtained from a single deposition in which *n*-type Ge was deposited on *p*-type GaAs (*n-p* junction) and on *n*-type GaAs, (*n-n* junction). The Ge was much more heavily doped than the GaAs. A combination of potential probing and thermoelectric probing[4] indicated that a potential barrier was present at the interface and that for both types of junctions the transition region was predominantly in the GaAs.

The junctions which were produced exhibited rectification properties. The rectification was of the opposite polarity for the two kinds of junctions. To bias the diodes to the low-resistance state (forward bias) it was necessary to bias the Ge negatively with respect to the GaAs for the *n-p* junctions and positively for the *n-n* junctions. In addition to these normally rectifying junctions, tunnel junctions have also been made.

Alignment of bands at interface

The "built-in" voltage (V_D) between the Ge and the GaAs was determined for these junctions by extrapolating the linear portion of the high current *V-I* characteristics to zero current. The built-in voltages for the *n-p* junction (V_D) and for the *n-n* junction (V_D') were found to be 0.62 ± 0.02 and 0.47 ± 0.02 v, respectively. These measurements indicate that the conduction and valence band edges are discontinuous at the junction by approximately 0.54 and 0.14 ev, respectively. This is shown in Fig. 1 for the situation where charge neutrality is assumed to exist at every point. This is not the band picture at equilibrium. The actual electrostatic profile for equilibrium depends on the doping in the materials. Figures 2 and 3 depict the equilibrium conditions for *n-p* and *n-n* heterojunctions, respectively. To obtain the values for the discontinuities at the interface, the published band gaps of 0.68 and 1.36 ev were assumed for Ge and GaAs, respectively, and it was further assumed that the Fermi level in the Ge coincided with the conduction band edge. Sheet resistivity measurements[5] indicate a net donor concentration in the Ge of about $10^{19}/cm^3$. At this impurity concentration, the assumptions as to the position of the Fermi level and the width of the forbidden band in Ge may not be valid, and so the discontinuities may not be exactly as indicated.

Figure 1 **Energy-band diagram for a Ge and GaAs heterojunction.**
Space-charge neutrality is assumed to exist at every point. This is the picture for high forward-bias where IR drops in the bulk semiconductor are neglected.



*This is a summary of a dissertation submitted in partial fulfillment of the requirements for the degree of Doctor of Philosophy in the Graduate School of Syracuse University, January 1960.

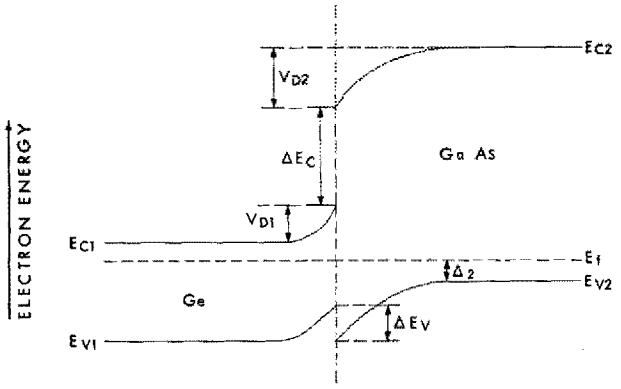


Figure 2 **Energy-band diagram for *n-p* heterojunction at equilibrium.**

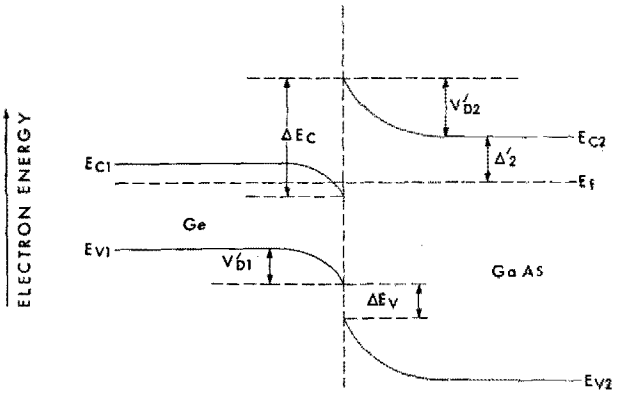


Figure 3 **Energy-band diagram for *n-n* heterojunction at equilibrium.**

In the absence of charged "interface states," the sum of the built-in voltages for the two kinds of junctions would be

$$V_D+V'_D=E_{g2}-\Delta_2-\Delta'_2\,, \tag{1}$$

where the symbols refer to Figs. 1, 2, and 3 and the built-in voltages V_D and V'_D are equal to the sums of the partial built-in voltages $V_{D1}+V_{D2}$ and $V'_{D1}+V'_{D2}$. The primed symbols refer to *n-n* junctions and the unprimed to *n-p* junctions.

Relationship (1) was verified within experimental error, and so the interface state density was not high enough to preclude agreement between theory and experiment. In the above expression, E_{g2} is the band gap in the GaAs. The values of Δ_2 and Δ'_2 (the energy differences between the conduction band edge and the Fermi level, and between the valence band edge and the Fermi level, for *n*- and *p*-type GaAs, respectively) were calculated using an effective mass for holes equal to the true electron mass (m) and the published value[6] of 0.078 m for the effective mass for electrons. These values of Δ_2 and Δ'_2 were found to be 0.19 and 0.07 ev, respectively.

Tunnel diodes have been made by depositing phosphorus-doped, degenerate *n*-type Ge on zinc-doped degenerate *p*-type GaAs.[3] A cross-sectional view is shown on page 246. The *V-I* characteristics of such a diode are shown in Fig. 4. The built-in voltage between the two materials was measured to be 0.90 ± 0.05 v, which is approximately what would be expected by the theory presented here.

Charge distribution

The conventional theory for homojunctions[1] of the electrostatic charge distribution and the differential capacitance, $C\equiv dQ/dV$, obtained by solving Poisson's equation for a space charge determined by local equilibrium, is readily generalized for heterojunctions. The most important results are given below and the experimental results for the transition capacity are related to theory.

For the *n-p* junctions, the space-charge density in the transition region is proportional to the net impurity density. For an abrupt junction, the depletion region width on the GaAs side (W_2) is for an applied voltage V

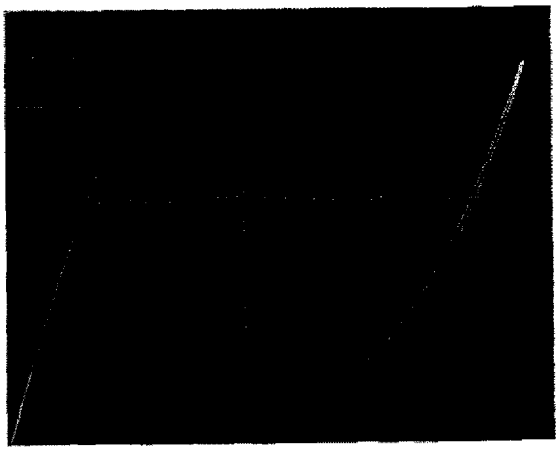
$$W_2=\left[\frac{2}{q}\,\frac{N_{D1}}{N_{A2}}\,\frac{\varepsilon_1\varepsilon_2(V_D-V)}{\varepsilon_1 N_{D1}+\varepsilon_2 N_{A2}}\right]^{1/2}, \tag{2}$$

where N_{D1} and ε_1 are the net donor concentration and the permittivity respectively for the Ge side, and N_{A2} and ε_2 are net acceptor concentration and permittivity on the GaAs side. A similar equation with an exchange of subscripts applies to the Ge side. The ratio of the fractions of the transition region width appearing on either side of the junction is

$$\frac{W_2}{W_1}=\frac{N_{D1}}{N_{A2}} \tag{3}$$

as in the case of an *n-p* homojunction.

Figure 4 **V-I characteristics of Ge-GaAs tunnel *n-p* heterojunction.**
The ordinate scale is 50 ma/div and the abscissa scale 0.1 v/div.



The relative potentials supported in each of the semiconductors are

$$\frac{V_{D1}-V_1}{V_{D2}-V_2}=\frac{N_{A2}\varepsilon_2}{N_{D1}\varepsilon_1}, \tag{4}$$

where V_1 and V_2 are the portions of the applied voltage appearing on the Ge side and on the GaAs side, respectively.

The transition capacitance for an abrupt n-p junction is given by a generalization of the usual result:

$$C_{n\text{-}p}=\left[\frac{qN_{D1}N_{A2}\varepsilon_1\varepsilon_2}{2(\varepsilon_1N_{D1}+\varepsilon_2N_{D2})(V_D-V)}\right]^{1/2}. \tag{5a}$$

The case of an n-n junction is somewhat different. The relative alignments of the Fermi levels with respect to the band edges are such that the space charge in the Ge region consists of mobile charge (electrons) in the conduction band. The solution to Poisson's equation in this case is tedious, but it is relatively easy to show that, except for very small values of V_D-V, the voltage drop is expected to be predominantly in the GaAs, and the capacitance is determined primarily by the characteristics of the GaAs. For a constant impurity density in the GaAs the transition capacitance is

$$C_{n\text{-}n}=\left[\frac{qN_{D2}\varepsilon_2}{2(V_D-V)}\right]^{1/2}. \tag{5b}$$

For the cases in which the impurity density varies with position, Eq. (5a) and (5b) are not applicable. If the capacitance can be expressed empirically as

$$C=C_1(V_D-V)^{-\alpha}, \tag{6}$$

a plot of V vs $(1/C)^{1/\alpha}$ extrapolated to a zero value of $(1/C)^{1/\alpha}$ gives the built-in voltage V_D.[7] From the values of C_1, α and junction area, the net ionized impurity concentration on the more lightly doped side of the junction can be obtained.[8] The values of α obtained experimentally are 0.5 and 0.15, and the values of V_D and V_D are 0.85 ± 0.05 and 0.50 ± 0.05 for n-p and n-n heterojunctions, respectively. This is probably not as accurate a method of determining V_D as the one described earlier, since it depends upon an extrapolation which assumes that the function describing the net impurity concentration in the GaAs with distance from the interface remains unchanged to the interface.

The value of α equal to 0.5 for the n-p heterojunction indicates that the acceptor concentration is a constant ($1.5\times10^{16}/\text{cm}^3$) in the region measured. The value of $V_D=0.85$ suggests, however, that the doping level becomes lighter near the interface. A variation in the doping level near the junction was observed in the n-n junctions. The value of $\alpha=0.15$ indicates a net donor concentration varying[8] as $X^{4.7}$, where X is the distance from the interface. The agreement between the value of V_D measured this way and from the V-I characteristics suggests that this relationship holds to the interface. It should be mentioned that lightly doped n-type GaAs seeds were converted to p-type near the interface and a p-n homojunction within the GaAs resulted. These units are not those reported on in this communication.

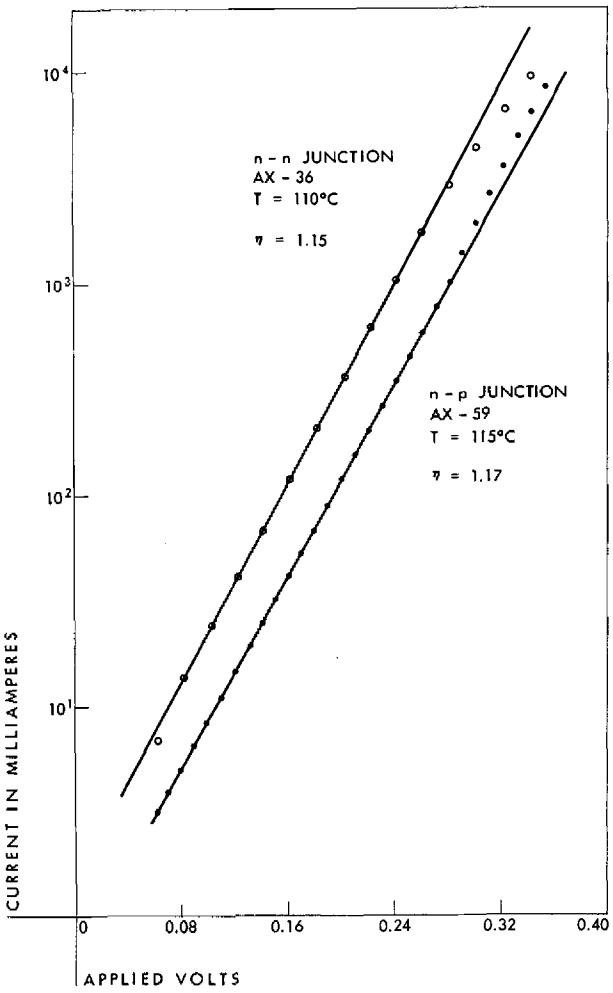


Figure 5 **Plot of ln I vs forward volts for n-n and n-p junctions at elevated temperatures. The values of η from Eq. (17) are indicated.**

V-I characteristics

The V-I characteristics at room temperature and at elevated temperatures show an exponential increase of current with forward voltage for both n-p and n-n heterojunctions. The current also increases approximately exponentially with reverse voltage for these junctions, although the increase is much more gradual than for the case of forward bias. Forward and reverse characteristics of two representative junctions are shown in Figs. 5 and 6, respectively. The elevated temperature data are shown because surface leakage is expected to be comparatively unimportant at these temperatures.

For the n-p heterojunction the current would be expected to be mainly by holes [the barrier for holes, (V_{D2}), is less than for electrons, ($V_{D2}+V_{D1}+\Delta E_C$)] and

would be expected to be given by the formula[9]

$$J_{n\text{-}p}=B\exp\left(-q\frac{V_{D2}}{kT}\right)\left[\exp\left(q\frac{V}{kT}\right)-1\right], \qquad (7)$$

where

$$B=qN_{A2}\sqrt{D_p/\tau_p}\,. \qquad (8)$$

Here D_p and τ_p are respectively diffusion constant and lifetime for holes in Ge.

The current in the *n-n* heterojunction would be expected to be carried by electrons which have sufficient energy to surmount the barrier (here the barrier for electrons is less than that for holes). Since the barrier width is about a mean free path, the emission theory[10] should apply, or

$$J_{n\text{-}n}=B'\exp\left(-q\frac{V'_{D2}}{kT}\right)\left[\exp\left(q\frac{V}{kT}\right)-1\right] \qquad (9)$$

where

$$B'=qN_{D2}\left(\frac{kT}{2m^*}\right)^{1/2}. \qquad (10)$$

Here N_{D2} is the donor concentration at the edge of the transition region and m^* is the electron effective mass in the GaAs.

For parameters B and B', it is assumed that all electrons which have sufficient momentum to surmount the barrier will pass over it.

If Eqs. (7) and (9) are applicable, it means that the potential barriers (V_{D2} and V'_{D2}) must decrease with an increase in reverse voltage for agreement with experimental characteristics, since B and B' are reasonably insensitive to applied voltage. The two most likely effects which could contribute to a lowering of the potential barriers with applied reverse voltage are image effects[11,12] and quantum-mechanical tunneling.[11]

The image effect is analogous to the Schottky effect in vacuum diodes. Because of the difference in permittivity in Ge and GaAs, the potential barrier would be expected to be lowered. The amount of lowering (ϕ_i) can be expressed

$$\phi_i=\left[\frac{qF_0}{4\pi\varepsilon'}\right]^{1/2}, \qquad (11)$$

where F_0 is the magnitude of the field strength at the interface, neglecting the image effect, and[13]

$$\varepsilon'=\varepsilon_2\frac{(\varepsilon_1+\varepsilon_2)}{(\varepsilon_1-\varepsilon_2)}.$$

The value of F_0 can be found from capacitance measurements (provided an extrapolation of Eq. (6) to zero value of V_D-V is valid) and is

$$F_0=\frac{C_1}{\varepsilon_2 A}\frac{(V_D-V)^{1-\alpha}}{(1-\alpha)}, \qquad (12)$$

where C_1 is the constant in Eq. (6) and A is the junction area.

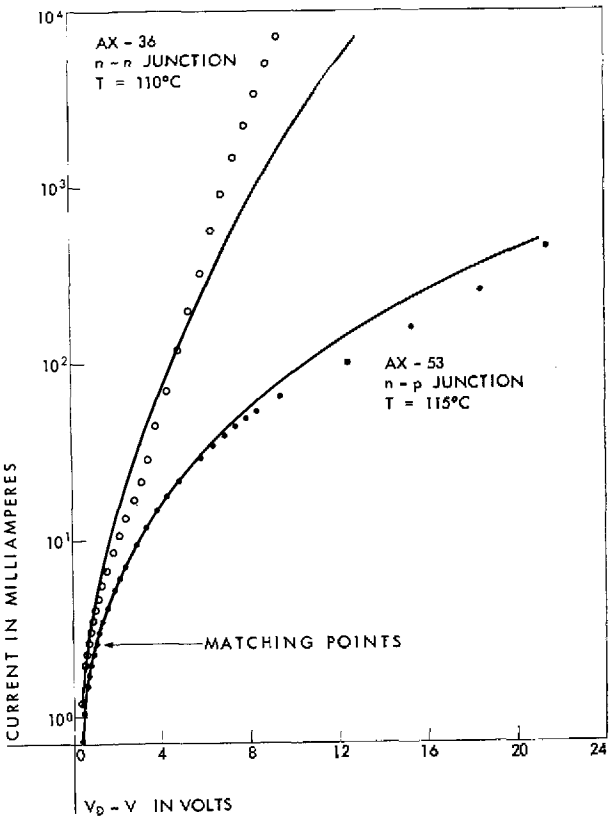


Figure 6 **Experimental points and theoretical curves for reverse *V-I* characteristics at elevated temperatures for *n-n* and *n-p* heterojunctions.**
Dots and circles are experimental data and solid lines are theoretical.

For the diodes discussed, F_0 is equal to 6×10^4 v/cm and 2×10^4 v/cm at equilibrium for *n-p* and *n-n* junctions respectively.

Hence

$$\phi_i=0.11(V_D-V)^{1/4} \quad \text{for } n\text{-}p \text{ junctions} \qquad (13a)$$

and

$$\phi'_i=0.087(V_D-V)^{0.43} \quad \text{for } n\text{-}n \text{ junctions,} \qquad (13b)$$

where ϕ_i is measured in electron volts.

If the effect of image forces on the barrier shape is neglected, the tunneling probability ($T(E)$) at any energy (E) below the top of the barrier for an *n-n* heterojunction is[14]

$$T(E)=\exp\left(-\frac{4}{3}\sqrt{\frac{2m^*q}{\hbar^2}}\frac{(E)^{3/2}}{F_0}\right). \qquad (14)$$

The same expression holds for a *n-p* junction if E is the energy above the bottom of the potential barrier.

The effective barrier-height reduction (ϕ_t) due to tunneling can be found by determining the current which tunnels and by equating this to the current which would flow over the barrier by a reduction in height of ϕ_t. This

can be obtained from the formula

$$\int_0^{\phi_t} \exp\left(q\frac{E}{kT}\right)dE = \int_0^{E_{max}} \exp\left(q\frac{E}{kT}\right)T(E)dE\,, \tag{15}$$

where E_{max} is the energy at the germanium valence and conduction band edges for *n-p* and *n-n* heterojunctions, respectively.

The correct value of m^* for Eq. (14) is difficult to determine, but if the value for GaAs is used and Eq. (15) is solved graphically to determine ϕ_t, then approximately

$$\phi_t = 0.020(V_D - V)^{0.42} \text{ for } n\text{-}p \text{ junctions at } 115°\text{C} \tag{16a}$$

and

$$\phi_t' = 0.019(V_D - V)^{0.63} \text{ for } n\text{-}n \text{ junctions at } 110°\text{C}. \tag{16b}$$

If the effect on barrier shape of image effects is considered, the values of ϕ_t would be somewhat smaller than those calculated.

If V_{D2} is replaced by $V_{D2}^{\circ} - \phi_i - \phi_t$ in Eq. (7) and V_{D2}' is replaced by $V_{D2}^{\circ\prime} - \phi_i' - \phi_t'$ in Eq. (9) (where V_{D2}° and $V_{D2}^{\circ\prime}$ are barrier heights for *n-p* and *n-n* junctions respectively, neglecting barrier depression), expressions which agree reasonably well with experiment are obtained. These "theory" curves are plotted in Fig. 6 along with experimental data. The theoretical and experimental curves are matched at the points shown. The theoretical curves were calculated assuming that any degree of barrier lowering is possible. Clearly, however, the maximum lowering permissible is ΔE_C and ΔE_V for *n-n* and *n-p* junctions respectively. Although the barrier lowering is considerably less than ΔE_C for the *n-n* junctions, the calculated value for *n-p* junctions is equal to ΔE_V(0.14 ev) for $V_D - V = 1.4$ v. It would be expected then, that the current in unit AX-53 (Fig. 6) would saturate at 3.5 μa. However, the agreement between theory (assuming no limit on barrier lowering) and experiment suggests that ΔE_V is greater than 0.14 ev. This may be because the band gap in Ge is less than 0.68 v for this degenerate Ge or because the effective discontinuity in the band edges is somewhat larger than the true value. This would be expected, since the discontinuities in the band edges and in the effective masses at the interface result in a high reflection coefficient of the Bloch waves describing carriers having energy just exceeding that of the barrier.

In the forward-bias condition the current density of a diode is often expressed as

$$J = J_0\left[\exp\left(q\frac{V}{\eta kT}\right) - 1\right], \tag{17}$$

where the experimental value of η is greater than unity. Experimental values of η for these junctions are indicated in Fig. 5. The value of η can be obtained from

$$\eta = \frac{q}{kT}\frac{dV}{d(\ln J)}. \tag{18}$$

Values of η equal to 1.18 and 1.12 are calculated for *n-p* and *n-n* junctions respectively at $(V_D - V) = 0.2$ volts by substituting Eqs. (7) and (9) (with barrier height corrected for tunneling and image effects) into Eq. (18). These values compare favorably with 1.17 and 1.15, which are the experimental values for these junctions.

Although the experimental curves agree reasonably well with Eqs. (7) and (9) for these junctions provided the values of B and B' are treated as "adjustable constants" (the curves in Fig. 6 are "matched"), the values of B and B' are respectively about three and six orders of magnitude too small for these *n-p* and *n-n* heterojunctions as calculated from Eqs. (8) and (10). This small value of current might be accounted for by the large reflection expected at the interface as a result of matching the incident, transmitted and reflected Bloch waves. The Bloch waves would be expected to be radically different in the two materials because of the differences in band structure and potential energy on either side of the interface.

Acknowledgments

The author wishes to thank Miss Anne Benoric, who fabricated the diodes for this study. Gratitude is also expressed to Miss M. J. O'Rourke and J. C. Marinace for help with the deposition process, and to P. J. Price, W. P. Dumke, J. C. Marinace, M. J. O'Rourke and J. A. Swanson for many helpful discussions.

References and footnotes

1. Junctions between two dissimilar semiconductors will be referred to as *heterojunctions* and those in the same semiconductor with different doping as *homojunctions*.
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Received April 25, 1960.