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SECURITY CLASSIFICATION OF THIS PAGE

AD-A177 254

REPORT DOCUMENTATION PAGE

1a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED		1b. RESTRICTIVE MARKINGS													
2a. SECURITY CLASSIFICATION AUTHORITY		3. DISTRIBUTION/AVAILABILITY OF REPORT Approved for public release; distribution unlimited.													
2b. DECLASSIFICATION/DOWNGRADING SCHEDULE															
4. PERFORMING ORGANIZATION REPORT NUMBER(S)		5. MONITORING ORGANIZATION REPORT NUMBER(S) AFOSR-TR- 87-0075													
6a. NAME OF PERFORMING ORGANIZATION SRI International	6b. OFFICE SYMBOL (If applicable)	7a. NAME OF MONITORING ORGANIZATION AFOSR													
6c. ADDRESS (City, State and ZIP Code) 333 Ravenswood Ave. Menio Park CA		7b. ADDRESS (City, State and ZIP Code) Bolling AFB DC Wash., DC													
8a. NAME OF FUNDING/SPONSORING ORGANIZATION AFOSR	8b. OFFICE SYMBOL (If applicable) NE	9. PROCUREMENT INSTRUMENT IDENTIFICATION NUMBER F49620-85-C-0103													
8c. ADDRESS (City, State and ZIP Code) 7b		10. SOURCE OF FUNDING NOS. <table border="1"><thead><tr><th>PROGRAM ELEMENT NO.</th><th>PROJECT NO.</th><th>TASK NO.</th><th>WORK UNIT NO.</th></tr></thead><tbody><tr><td>61102f</td><td>5396</td><td>00</td><td>DARPA</td></tr></tbody></table>		PROGRAM ELEMENT NO.	PROJECT NO.	TASK NO.	WORK UNIT NO.	61102f	5396	00	DARPA				
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61102f	5396	00	DARPA												
11. TITLE (Include Security Classification) Semiconductor Engineering for High Speed Devices															
12. PERSONAL AUTHOR(S) SHER															
13a. TYPE OF REPORT 5th Quarterly Status Rpt	13b. TIME COVERED FROM 6-14-86 TO 9-15-86	14. DATE OF REPORT (Yr., Mo., Day) 15 Oct 86	15. PAGE COUNT 14												
16. SUPPLEMENTARY NOTATION															
17. COSATI CODES <table border="1"><thead><tr><th>FIELD</th><th>GROUP</th><th>SUB. GR.</th></tr></thead><tbody><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr><tr><td></td><td></td><td></td></tr></tbody></table>		FIELD	GROUP	SUB. GR.										18. SUBJECT TERMS (Continue on reverse if necessary and identify by block number)	
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19. ABSTRACT (Continue on reverse if necessary and identify by block number) 14 June 1987 This report summarizes major accomplishments covering the period 15 June to 15 September 1986. The results are discussed in four sections: Section I Describes CPA calculations of the group velocity and the mean free path. These numbers are needed to design ballistic transport devices. We have determined the optimum injection angles and energies for several of the most promising alloys. Calculations of the effect of anisotropy and intervalley scattering mediated by ionized impurities on v-E characteristic are described in Section II. Based on the more accurate evaluations of the band structures, and alloy and impurity scattering, we suggest promising candidate materials for high-speed devices. Section III is a concise statement of SRI's conclusions and recommendations. Section IV is devoted to administrative matters.															
20. DISTRIBUTION/AVAILABILITY OF ABSTRACT UNCLASSIFIED/UNLIMITED ☐ SAME AS RPT. ☐ DTIC USERS ☐		21. ABSTRACT SECURITY CLASSIFICATION UUUUU													
22a. NAME OF RESPONSIBLE INDIVIDUAL Kevin Malloy		22b. TELEPHONE NUMBER (Include Area Code) 767-4931	22c. OFFICE SYMBOL NE												

SRI International



AFOSR-TR. 87-0075

SEMICONDUCTOR ENGINEERING FOR HIGH-SPEED DEVICES

Quarterly R&D Status Report 5

Covering the Period 14 June 1986 to 15 September 1986

15 October 1986

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ARPA Order 5396, Program Code 5D10
Contract F49620-85-C-0103
Effective Date: 1 June 1985
Contract Expiration Date: 31 May 1988
Contract Dollars: \$611,296

SRI Project 8725

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DESCRIPTION OF PROGRESS

This report summarizes major accomplishments covering the period 15 June to 15 September 1986.

The results are discussed in four sections:

- Section I describes CPA calculations of the group velocity and the mean free path. These numbers are needed to design ballistic transport devices. We have determined the optimum injection angles and energies for several of the most promising alloys.
- Calculations of the effect of anisotropy and intervalley scattering mediated by ionized impurities on v-E characteristic are described in Section II. Based on the more accurate evaluations of the band structures, and alloy and impurity scattering, we suggest promising candidate materials for high-speed devices.
- Section III is a concise statement of SRI's conclusions and recommendations.
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I CALCULATION OF GROUP VELOCITY AND MEAN FREE PATH

Group velocities v_g based on VCA band structures were presented in our last report. In this period we have used the CRAY computer to carry out full CPA evaluations of the band structure and alloy scattering rates including both diagonal and off-diagonal disorder for the most promising alloys $\text{Ga}_{1-x}\text{In}_x\text{As}$ and $\text{InP}_{1-x}\text{As}_x$. Because this procedure automatically incorporates anisotropic intervalley scattering, we are able to calculate the group velocity and mean free path for electrons launched into the alloy medium with various energies in different crystallographic directions. We are now adding phonon and impurity scattering to complete this picture. The variation of these self energies with $\vec{k}$ in the Brillouin zone are useful to the specialist; we do not include curves in this report because they are not of direct concern in device design. Rather, we combine the self energies with the group velocity to calculate the alloy-scattering-limited mean free path.

Figure 1 shows the group velocities $\vec{v}_g = 1/\hbar \nabla_{\vec{k}} \epsilon(\vec{k})$ for the conduction band states of several alloys, $\text{Ga}_{1-x}\text{In}_x\text{As}$ ($x = 0.5, 0.75$), $\text{InP}_{1-x}\text{As}_x$ ($x = 0.5$) for $\vec{k}$ in the ΓX and ΓL directions. In all cases the group velocity reaches its maximum values in the ΓX (1,0,0) direction. Similar results have been found for the pure compounds GaAs, GaSb, InP, InAs, and InSb [see Status Report 4 (13 June 1986)]. Notice that the peak values of v_g in the ΓX direction are 12.1, 8.9, 11.6, 14.8, and 12.1 [10^7 cm/s], respectively. The value of v_g in GaSb is smaller than for the other alloys; otherwise, there is relatively little to choose among the others except for InAs. The best of the lot is InAs, but the band gap of this material is relatively small for it to be a practical choice for a room-temperature device.

In Figures 2 and 3, the mean free path due to alloy scattering λ_{alloy} , acoustic phonons λ_{ap} , and longitudinal optical phonons λ_{op} are presented and combined into a total mean free path, λ , as follows:

$$\lambda^{-1} = \lambda_{\text{alloy}}^{-1} + \lambda_{\text{ap}}^{-1} + \lambda_{\text{op}}^{-1} .$$

Acoustic phonons never dominate. Optical phonons are dominant at low momenta (energies) and alloy-mediated intervalley scattering becomes dominant at higher momenta. Near the v_g peak, the mean free path drops to troublesome low values of a few hundred angstroms. Thus, it may be necessary to inject the electrons with momenta slightly smaller than those corresponding to the highest v_g to achieve a sufficiently long mean free path for a practical device.

To emphasize this point in terms corresponding to actual experimental arrangements, we have replotted in Figure 4 the group velocity and mean free path as a function of the injected electron energy. All of these plots assume the electrons are injected in the (1,0,0) direction.

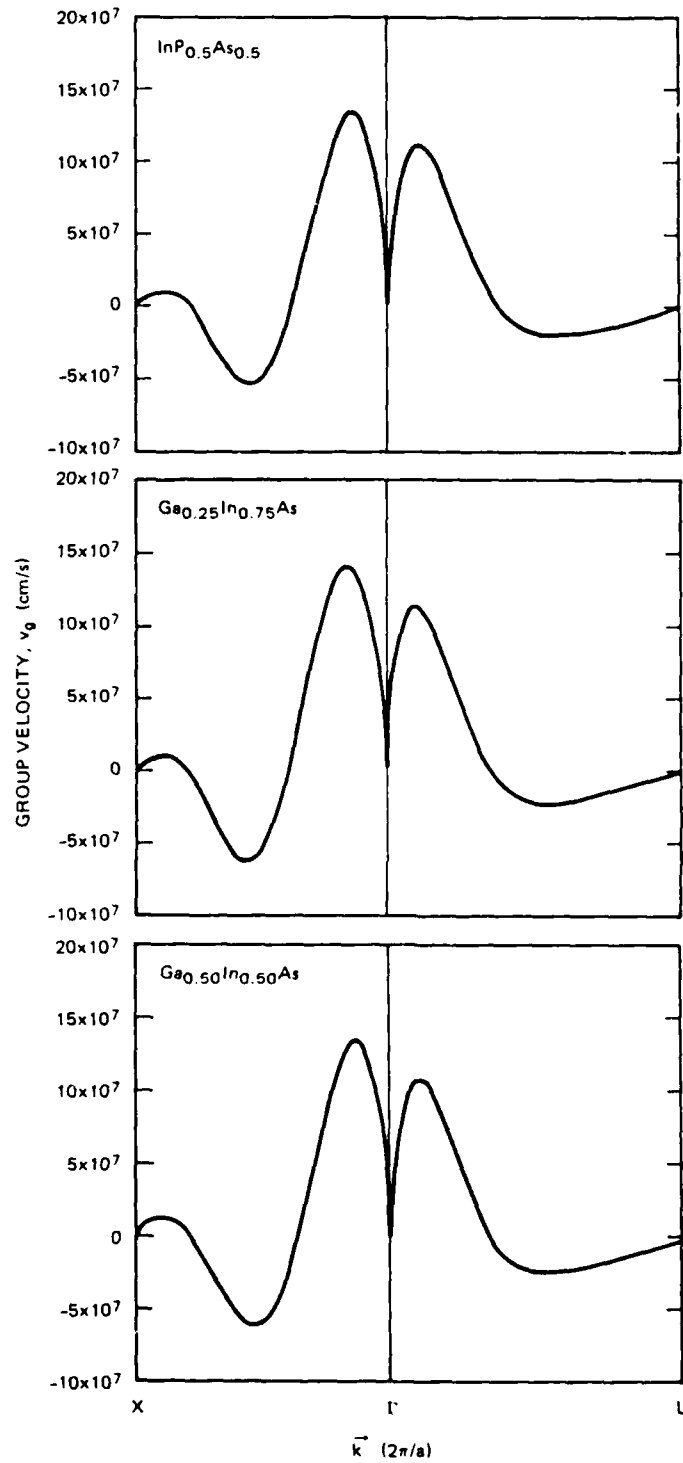


FIGURE 1 GROUP VELOCITY v_g IN ΓX , ΓL DIRECTIONS
IN $\text{InP}_{0.5}\text{As}_{0.5}$, $\text{Ga}_{0.25}\text{In}_{0.75}\text{As}$,
AND $\text{Ga}_{0.50}\text{In}_{0.50}\text{As}$ ALLOYS

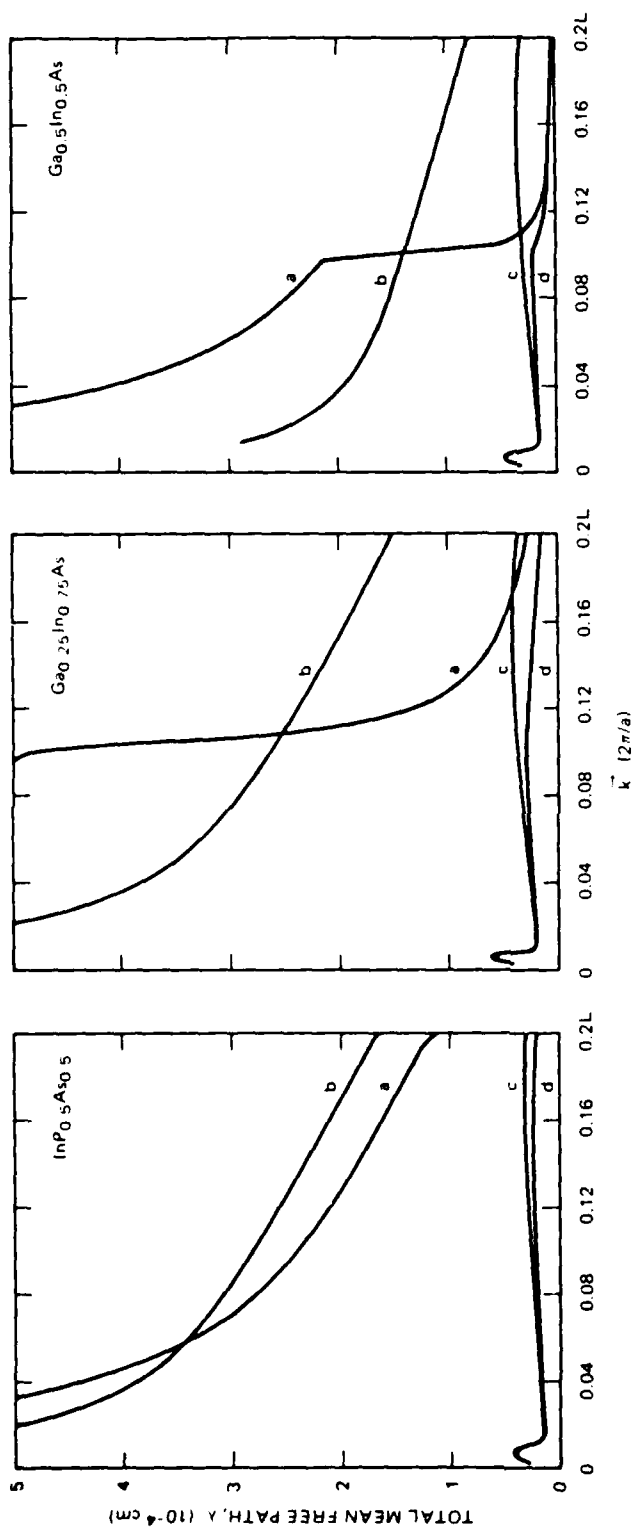


FIGURE 2 MEAN FREE PATH IN $\text{InP}_{0.5}\text{As}_{0.5}$, $\text{Ga}_{0.25}\text{In}_{0.75}\text{As}$, AND $\text{Ga}_{0.5}\text{In}_{0.5}\text{As}$ ALLOYS AS A FUNCTION OF $\vec{k}$ IN ΓL DIRECTION

Limitations imposed by alloy (a), acoustic phonon (b) and LO-phonon (c); (d) shows effective λ .

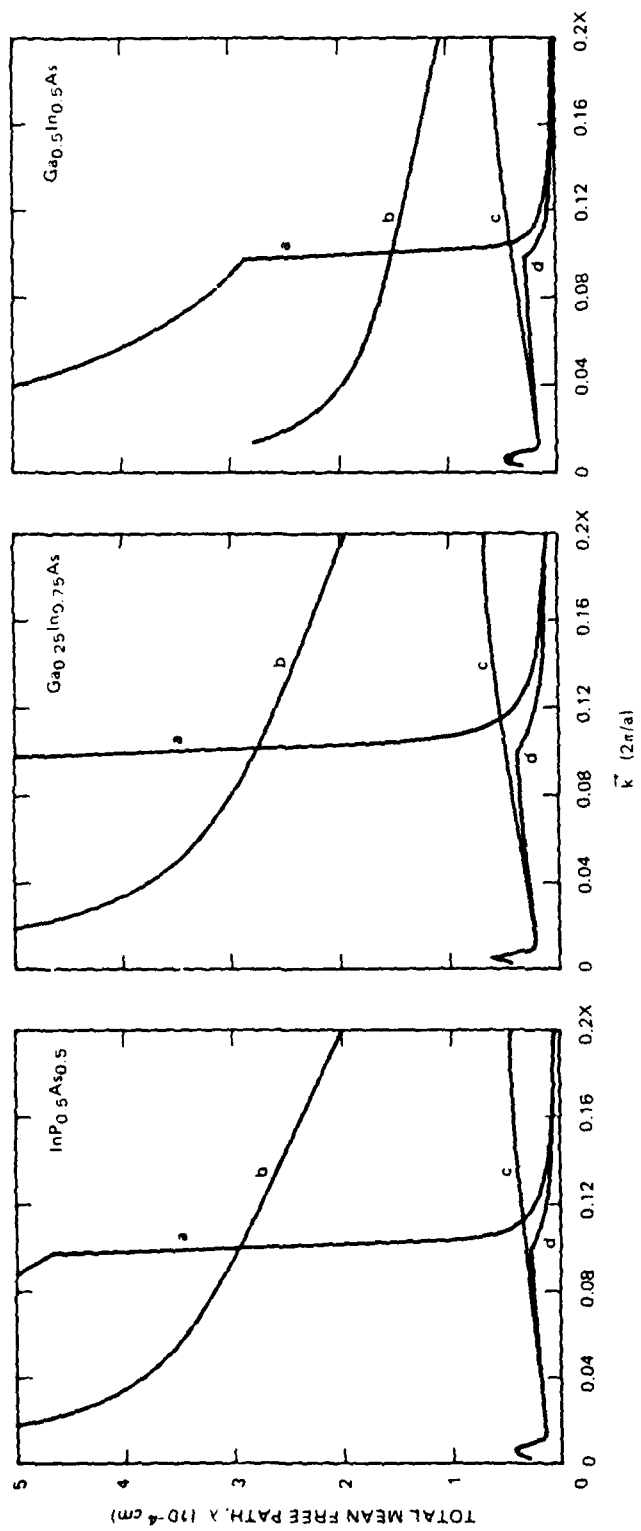


FIGURE 3 MEAN FREE PATH IN $\text{InP}_{0.5}\text{As}_{0.5}$, $\text{Ga}_{0.25}\text{In}_{0.75}\text{As}$, AND $\text{Ga}_{0.5}\text{In}_{0.5}\text{As}$ ALLOYS AS A FUNCTION OF $\vec{k}$ IN ΓX DIRECTION

Limitations imposed by alloy (a), acoustic phonon (b) and LO-phonon (c); (d) shows effective λ .

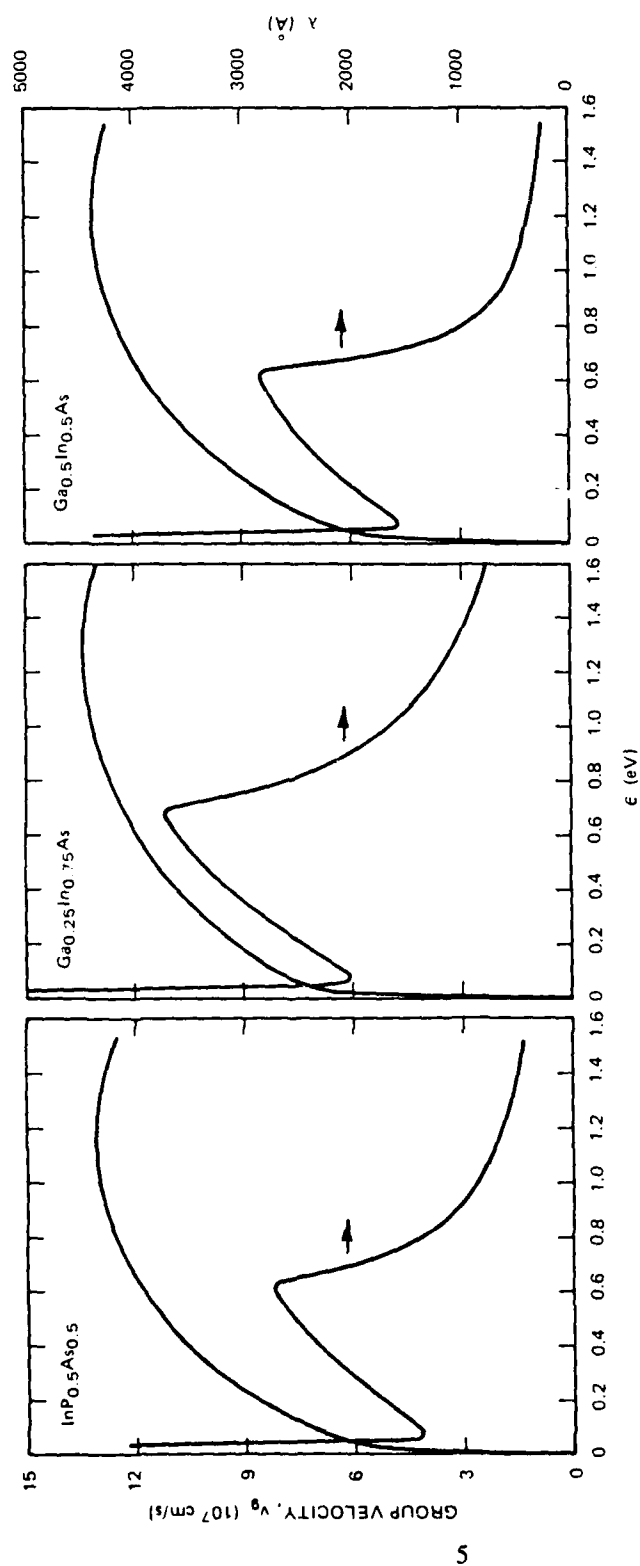


FIGURE 4 GROUP VELOCITY AND EFFECTIVE MEAN FREE PATH AS A FUNCTION OF ENERGY IN $\text{InP}_{0.5}\text{As}_{0.5}$, $\text{Ga}_{0.25}\text{In}_{0.75}\text{As}$, AND $\text{Ga}_{0.5}\text{In}_{0.5}\text{As}$ ALLOYS

Among the alloys studied, $\text{Ga}_{0.5}\text{In}_{0.5}\text{As}$ and $\text{InP}_{0.5}\text{As}_{0.5}$ both have maximum group velocities of approximately 13.0×10^7 cm/s. This is not appreciably higher than the group velocity for pure GaAs. We therefore conclude that, for ballistic transport devices, the pure compounds have electronic properties that are as good or better than those of any alloy. Thus, in this application, any use of alloys would be motivated by other considerations (e.g. larger elastic constants, reduced dislocation densities, a tailored band gap, or lattice constant matching).

II CALCULATION OF v-E CHARACTERISTICS

Another major accomplishment achieved in this period has been to include various anisotropy and intervalley scattering contributions to the drift velocity. Frequently, coupling constants for these mechanisms are fitted to obtain qualitative results. In our calculations, these coupling constants are evaluated directly from band structures. Computational complexity arises once the scattering is anisotropic, because the usual BZ sum, in which the integration is performed in only 1/48 of the BZ, is no longer valid. What would otherwise be tedious and time-consuming anisotropic calculations have been done on the CRAY computer.

Moreover, the momentum relaxation time that results from ionized impurity scattering, along with the electron's mobility μ_1 , have also been calculated. Figure 5 compares our results with the effective mass approximation (Smith, *Semiconductors*, 2nd ed. 1980, p. 257). The deviation at higher temperature is owing to departure from the parabolic form and intervalley scattering that are included in our calculations. For impurity densities, N_I , less than $10^{17}/\text{cm}^3$, the impurity scattering does not affect v-E curves substantially. Effects of impurity scattering for larger densities ($N_I = 10^{18}/\text{cm}^3$) on v-E graphs are clearly seen in Figure 6. Because the impurity scattering is more effective on low-energy electrons, the v-E curve deviates most at low $\vec{E}$. As the low-field mobility is decreased, the v_p decreases and ϵ_p increases. We see that impurity scattering is not effective at fields of approximately 10 kV/cm. However, at still higher fields, we expect it to be more effective because of intervalley scattering.

In the absence of impurity scattering, and with phonon scattering still added in an approximate way, the peak drift velocities v_p and the corresponding field E_p are listed in Table 1 for some reference compounds and for the more promising alloys. Actually InAs is not a realistic possibility, because its band gap is too narrow for use at room temperature. Notice that both $\text{Ga}_{0.5}\text{In}_{0.5}\text{As}$ and $\text{InP}_{0.5}\text{As}_{0.5}$ have significantly higher peak drift velocities than GaAs (1.6 and 1.9 times, respectively). Moreover, the fields (and therefore the power dissipated at the peak velocity) for the alloys are smaller than for pure GaAs. These alloys have only slightly higher peak drift velocities than InP; thus, by this measure of device performance, the extra trouble of growing the alloys would not be warranted. However, the values of E_p for both alloys lie well below that of InP; hence, the power dissipation in the alloys should be substantially lower than that in InP. A more quantitative conclusion will be offered when we have added the phonon scattering in a more complete treatment (which will give us greater assurance of the calculated velocity peak-to-valley ratios). In addition, we must still examine the properties of the $\text{InS}_{0.5}\text{As}_{0.5}$ alloy. While the bond length difference between InP and InSb are large enough to make it difficult to grow concentrated alloys, our preliminary results indicate that the material (if it can be prepared) will have favorable electronic properties.

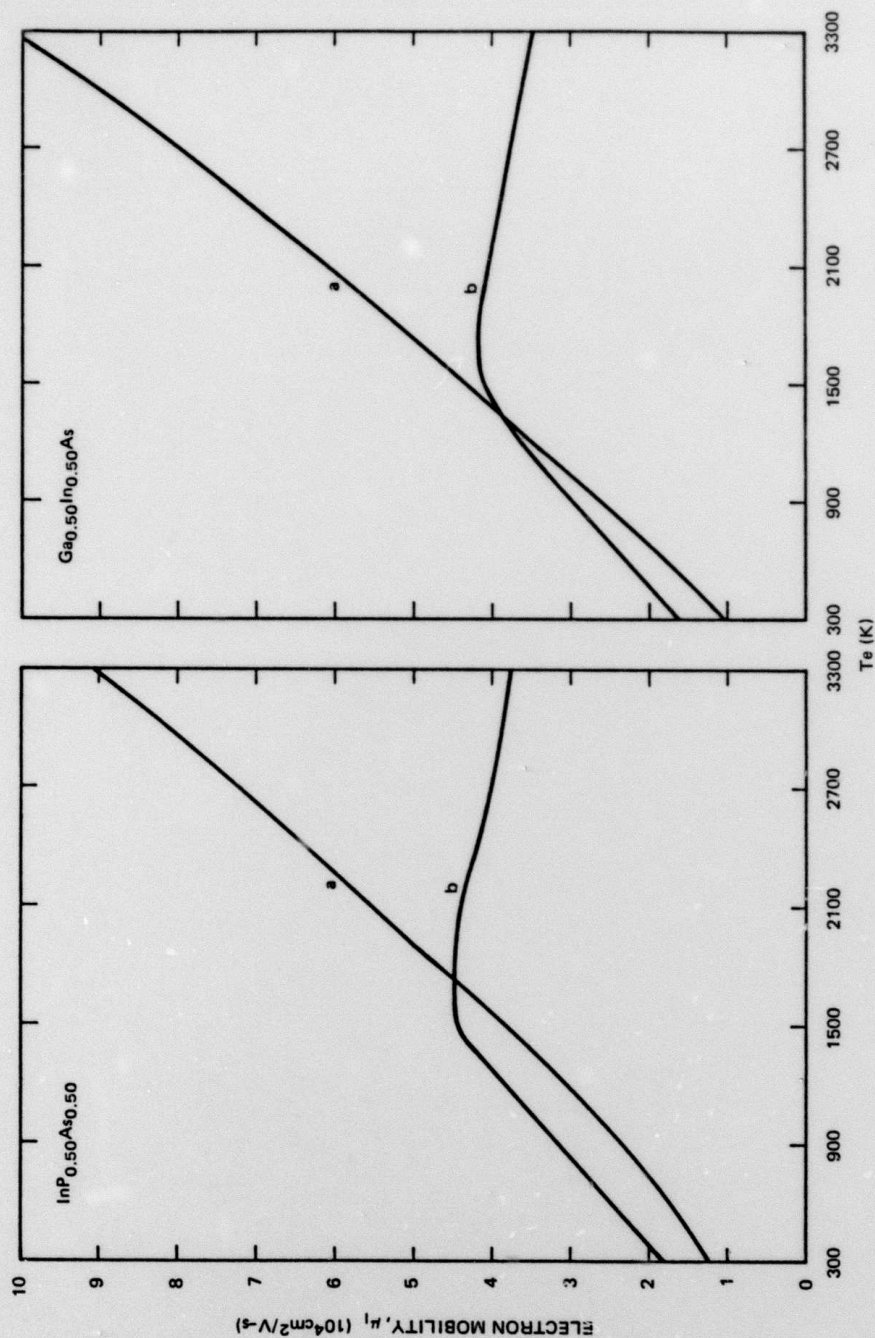


FIGURE 5 IMPURITY-SCATTERING-LIMITED ELECTRON MOBILITY AS A FUNCTION OF ELECTRON TEMPERATURE IN (a) EFFECTIVE MASS APPROXIMATION AND (b) OUR CALCULATIONS FOR $\text{InP}_{0.50}\text{As}_{0.50}$ AND $\text{Ga}_{0.50}\text{In}_{0.50}\text{As}$ ALLOYS

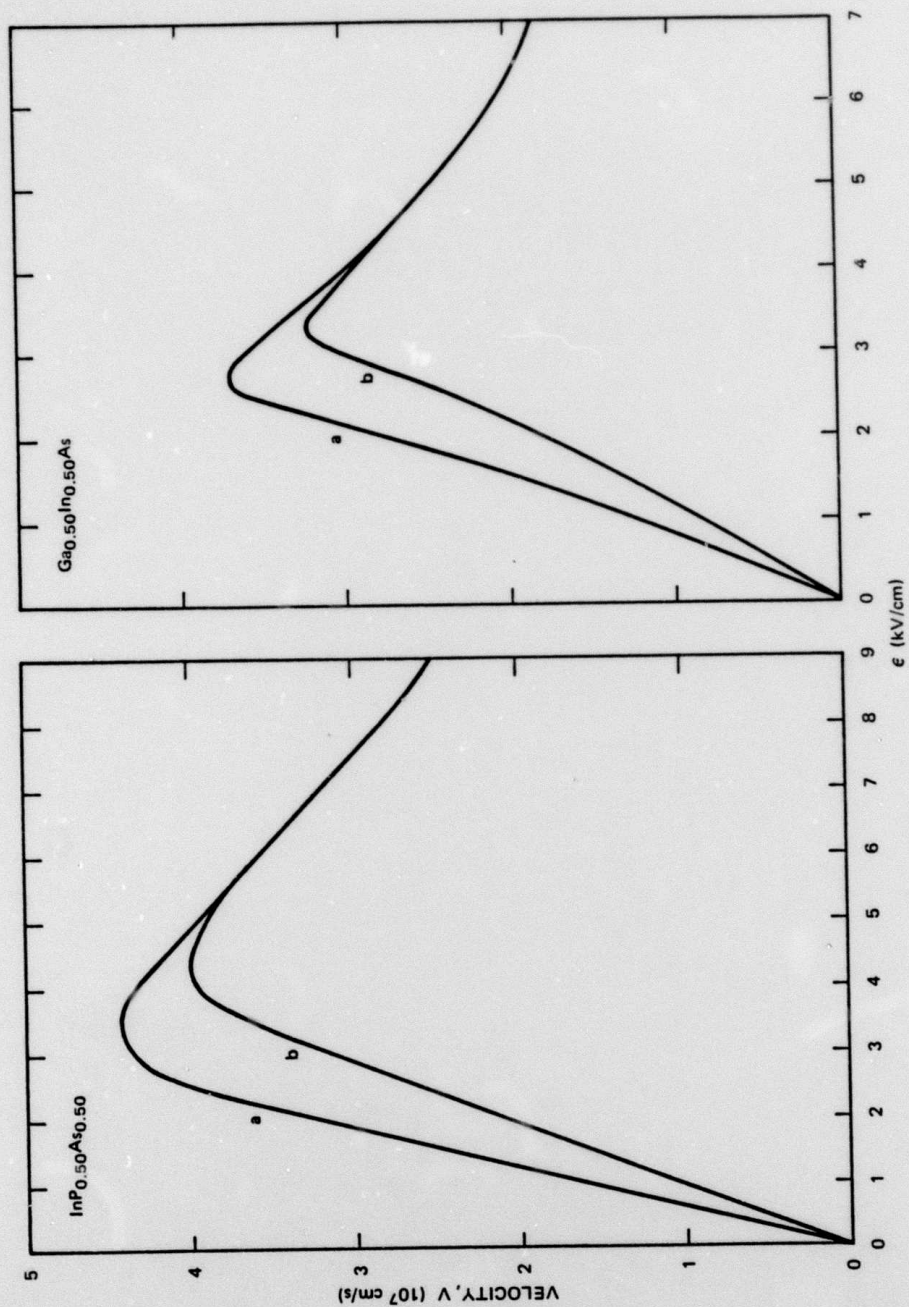


FIGURE 6 (a) ALLOY-SCATTERING-LIMITED AND (b) ALLOY-AND-IMPURITY-SCATTERING-LIMITED v-E CURVES AS SHOWN BY $\text{In}_{0.50}\text{As}_{0.50}$ AND $\text{Ga}_{0.50}\text{In}_{0.50}\text{As}$ AT $T = 300\text{K}$, $n_i = 10^{18}\text{cm}^{-3}$

Table 1

PEAK DRIFT VELOCITY AND CORRESPONDING FIELD

Compound	Peak Drift Velocity v_p (10^7 cm·s)	Field at Peak E_p (kV/cm)
GaAs	2.3	4
InAs	4.2	1.5
InP	3.6	8.0
Ga _{0.5} In _{0.5} As	3.7	2.8
InP _{0.5} As _{0.5}	4.4	3.5

III CONCLUSIONS AND RECOMMENDATIONS

We draw somewhat different conclusions about the utility of alloys in ballistic and drift transport dominated devices:

- For ballistic transport devices:
 - Direct gap materials are best.
 - Electrons should always be injected in the (1,0,0) direction. The next best direction, is the (1,1,0) followed by the (1,1,1).
 - GaAs, InP, and InAs have about equally high peak group velocities, and all can function at room temperature (although InAs is marginal).
 - No alloy has an appreciably higher peak group velocity than the pure compounds identified above.
 - If alloys are chosen, the decision will be made on the basis of properties other than maximum speed.
- Conclusions regarding drift transport devices are somewhat tentative because the way phonons are included requires further improvement; however:
 - All favorable alloys have constituents with direct band gaps.
 - Both $\text{Ga}_{1-x}\text{In}_x\text{As}$ and $\text{InP}_{1-x}\text{As}_x$ have distinct advantages over the most favorable pure compounds (GaAs, InP, and InAs).
 - The $\text{InP}_{1-x}\text{As}_x$ alloy may be somewhat less sensitive to charged impurity scattering than $\text{Ga}_{1-x}\text{In}_x\text{As}$. (This is the start of a study of nonideal effects.)

IV ADMINISTRATIVE INFORMATION

A. *Equipment Purchased or Constructed*

None.

B. *Trips, Meetings, Papers, and Visits*

Drs. Arden Sher and Srinivasan Krishnamurthy attended the International Conference on Semiconductor Alloys in Snowmass, Colorado, 15 September 1986.

C. *Problems or Areas of Concern*

None.

D. *Deviation from Planned Effort*

None.

E. *Fiscal Status*

The total contract funding for the three year period is \$611,296. Of this, \$195,287 was allocated to the first year. Including the burden, approximately \$22,000 was intended to pay the consulting fee of An-Ban Chen, leaving approximately \$173,000. In the first year ending 31 May 1986, we spent approximately \$192,000. Year Two has been allocated \$203,655 with \$20,284 intended to pay the consulting fee of An-Ban Chen. During the first quarter of Year Two (1 June to 31 August 1986), \$49,000 was spent.