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**THEORETICAL PREDICTION OF THE PLASMA FREQUENCY AND  
MOSS-BURSTEIN SHIFTS FOR DEGENERATELY DOPED  $\text{In}_x\text{Ga}_{1-x}\text{As}$**

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J. E. Reynolds, G. W. Charache

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KAPL ATOMIC POWER LABORATORY

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# Theoretical Prediction of the Plasma Frequency and Moss-Burstein Shifts for Degenerately Doped $\text{In}_x \text{Ga}_{1-x} \text{As}$

**J.E. Reynolds\***, **C.B. Geller\*\***, **G.W. Charache\***, **T. Holden\*\*\*** and **F.H. Pollak\*\*\***

\*Lockheed Martin Corp., Schenectady, NY

\*\*Bettis Atomic Power Laboratory, West Mifflin, PA

\*\*\*Physics Dept. and NYS Center for Advanced Technology in Ultrafast Photonic and Materials Applications, Brooklyn College of CUNY, Brooklyn, NY 11210

## 1. Abstract

Theoretical predictions for the plasma frequency and Moss-Burstein shift (optical band gap) of degenerately doped ( $n > 10^{19} \text{ cm}^{-3}$ )  $\text{In}_x \text{Ga}_{1-x} \text{As}$  are presented. This system is of interest because it possesses desirable optical properties for thermophotovoltaic (TPV) applications. The studies presented are based on electronic band structures calculated using the Full Potential Linearized Augmented Plane Wave (FLAPW) method which includes non-local screened exchange (sX-LDA) and spin-orbit effects. The plasma frequency and Moss-Burstein shift are calculated vs. doping assuming a "rigid band" approximation (i.e. conduction band filling of the "undoped" bands). The doping dependence of the effective mass (band non-parabolicity) plays an important role at the high dopings considered here. This effect leads to a maximum in the plasma frequency vs. doping ( $2 - 3 \times 10^{14} / \text{s}$ ) and a significant departure from the "constant effective mass" prediction for the optical band gap vs. doping. These calculations are in good agreement with measurements.

## 2. Introduction

In order to achieve the highest performance of TPV systems, spectral control filters are used to block radiation in regions of the black-body spectrum which cannot be converted to electricity. The long wavelength portion of the spectrum can be blocked by the use of a "plasma filter" which is a heavily doped semiconductor exhibiting metallic-like reflectivity at long wavelengths. Currently, InGaAs and InPAs alloys are being investigated experimentally as promising candidate materials for plasma filters.

Theoretical investigations were undertaken to resolve certain puzzling aspects of the measured doping dependence of the plasma frequency (frequency below which reflectivity becomes large) and the optical absorption edge. Classical theory predicts that the plasma frequency should increase linearly with the square root of the doping density, while measurements show that it actually saturates at high doping densities (on the order of  $10^{19} \text{ cm}^{-3}$ ). This discrepancy is due to the fact that the effective mass of charge carriers is not constant as assumed by the classical theory, but rather increases with doping. The Moss-Burstein shift (doping induced shift of the optical absorption edge) is also

affected by the fact that the carrier effective mass depends on doping.

### 3. Theoretical prediction of the plasma frequency and Moss-Burstein shift vs. doping

A theoretical description of the plasma frequency and Moss-Burstein shift requires an accurate band structure. To this end, we have carried out band structure calculations using the Full Potential Linear Augmented Plane Wave (FLAPW) method<sup>1</sup> which uses a hybrid Screened Exchange/Local Density Approximation (sX-LDA) functional to describe exchange correlation effects. This method has been shown to yield realistic semiconductor band gaps and conduction band dispersions.<sup>2</sup> The Moss-Burstein shift and plasma frequency are calculated from the FLAPW band structures in a rigid band picture. The Moss-Burstein shift is calculated by filling the conduction band (calculated for the undoped system) to a given energy, then determining the corresponding carrier density as

$$\rho = \frac{V_k}{(2\pi)^3}, \quad (\text{EQ 1})$$

where  $V_k$  is the corresponding volume in  $k$  space. A simple approximation is employed to determine  $V_k$ . The FLAPW bands along high symmetry directions are fit to polynomial expansions. A spherical average is then carried out to yield a one dimensional  $E$  vs.  $k$  relation:  $E = E(k)$ . The  $k$  space volume is then simply given by the volume of a sphere:

$$V_k = \frac{4\pi k^3}{3}. \quad (\text{EQ 2})$$

The plasma frequency is determined as the frequency for which the dielectric function:

$$\epsilon(\omega) = \epsilon_\infty - \frac{4\pi e^2}{\hbar^2 \omega^2} \int_0^{k_F} \frac{\partial^2 E}{\partial k^2} \frac{2}{(2\pi)^3} d\vec{k}, \quad (\text{EQ 3})$$

vanishes (working in cgs units).<sup>3</sup> In the previous equation  $e$  is the electron charge,  $\hbar$  is Planck's constant,  $\epsilon_\infty$  is the high frequency component of the dielectric function (the electronic interband part), and  $\omega$  is the angular frequency of electromagnetic wave. Thus, the plasma frequency  $\omega_p$  is given by:

$$\omega_p^2 = \frac{4\pi e^2}{\epsilon_\infty \hbar^2} \int_0^{k_F} \frac{\partial^2 E}{\partial k^2} \frac{2}{(2\pi)^3} d\vec{k}. \quad (\text{EQ 4})$$

This integral is evaluated in a manner similar to that for the Moss-Burstein shift. The bands are spherically averaged and the carrier density is proportional to the  $k$  space volume (the volume of a sphere). A doping dependent effective mass,  $m_s$ , can be defined in

terms of the dielectric function in the standard way:

$$\epsilon(\omega) = \epsilon_{\infty} - \frac{4\pi e^2 N}{\omega^2 m_s m_0} \quad (\text{EQ 5})$$

where  $N$  is the carrier density, and  $m_0$  is the electron mass. This effective mass,  $m_s$ , should not to be confused with the effective mass,  $m^*$ , of an electron in a given electronic state. Rather  $m_s$  represents the collective behavior of the conduction electrons. At high doping levels,  $m_s$  can become negative. The plasma frequency is undefined when the mass becomes negative because there is no solution to  $\epsilon(\omega) = 0$  for real frequencies. This implies that there is no plasma mode for sufficiently high dopings in this model.

#### 4. Results

The results for the plasma frequency of InGaAs vs. doping are presented in Fig. 1 along with measurements. These calculations are consistent with the observed saturation of the plasma frequency. The predicted decrease in the plasma frequency at high doping is not observed because the doping solubility limit is reached. The decrease in the plasma frequency at high doping results from the fact that the effective mass  $m^*$  (mass of an individual state) becomes negative above half filling of the band. The change in sign of the effective mass is due to the change in sign of the curvature of the bands. The states in the upper half of the band are of "anti-bonding" character. Therefore, there may be a connection between the solubility limit and band structure in that dopant atoms may be more likely to go into interstitial sites rather than to fill anti-bonding states, by going into substitutional sites.

The calculated results for the doping dependence of the optical absorption edge (Fermi energy) are presented in Fig. 2 along with experimental measurements. Also included in this figure is the prediction obtained assuming a constant effective mass (parabolic approximation for the conduction band dispersion). The calculated result increases more slowly with doping than the parabolic approximation (constant effective mass) predicts, due to the increase in effective mass with doping. The measured doping dependence of the Fermi energy is also consistent with an effective mass that increases with doping. The calculations were carried out for a system with composition In(0.75) Ga(0.25) As, while the measurements were performed on a system with In(0.66) Ga(0.33) As (numbers represent mole fractions). The composition for the calculation was chosen as it allows small unit cells to be used (8-atoms), thus greatly reducing the computational cost. The calculated band gap is thus smaller than the measured band gap due to this composition difference. A rigid shift of the calculated results to correct for this band gap would improve the agreement with the measurements.

In both Figs. 1 and 2, theoretical results are presented for the ideal atomic structures (minimum energy configuration with ideal interatomic separations) and the relaxed (lowest energy) atomic structure. Also, in both figures, the effect of relaxation (allowing bond lengths to change) is small and does not change the qualitative conclusions.

## 5. Conclusions

The present investigation helped to resolve the interpretation of experimental data that was in conflict with the predictions of simple classical theory. The calculations are in agreement with experiments in which a saturation of the plasma frequency with doping was observed. The classical theory, on the other hand, predicts the plasma frequency to increase as the square root of the doping density. The calculated shift of the optical absorption edge (to higher frequencies) vs. doping (Moss-Burstein shift) is also in better agreement with the experiments than is the classical prediction. The failure of the classical theory is due to the fact that it does not account for the doping dependence of the effective mass of the charge carriers.

### Figures:

Figure 1. Calculated plasma frequency vs. doping density for InGaAs along with experimental measurements. The calculation is based on the composition In(0.75) Ga(0.25) As and was chosen because it allows the use of a small unit cell (8-atoms). The composition for which measurements were made was In(0.66) Ga(0.33) As. The atomic configuration used in the calculation is the one giving the minimum energy assuming ideal inter atomic separation. Results are also present for the configuration in which the inter atomic separations were allowed to relax. These calculations are consistent with the observed saturation of the plasma frequency.

Figure 2. Calculated Fermi level vs. doping density for InGaAs along with experimental measurements and parabolic band prediction (see Fig. 1 caption for details of the calculation). The discrepancy between the experiment and the calculation at low doping is largely due to the fact that the composition chosen for the calculation differs from that of the experiment (see Fig. 1 caption). The doping dependent effective mass is evident from the fact that the Fermi energy increases with doping more gradually than predicted by the parabolic band approximation (constant effective mass).

### References:

1. H. J. F. Jansen and A. J. Freeman, Phys. Rev. B 30, 561 (1984).
2. C.B. Geller and T.S. Blazek, 4th NREL conference on TPV, session #1, talk #5.
3. W. G. Spitzer and H. Y. Fan, Phys. Rev. 106, 882 (1957).

# In(0.75) Ga(0.25) As: Plasma frequency vs. carrier density

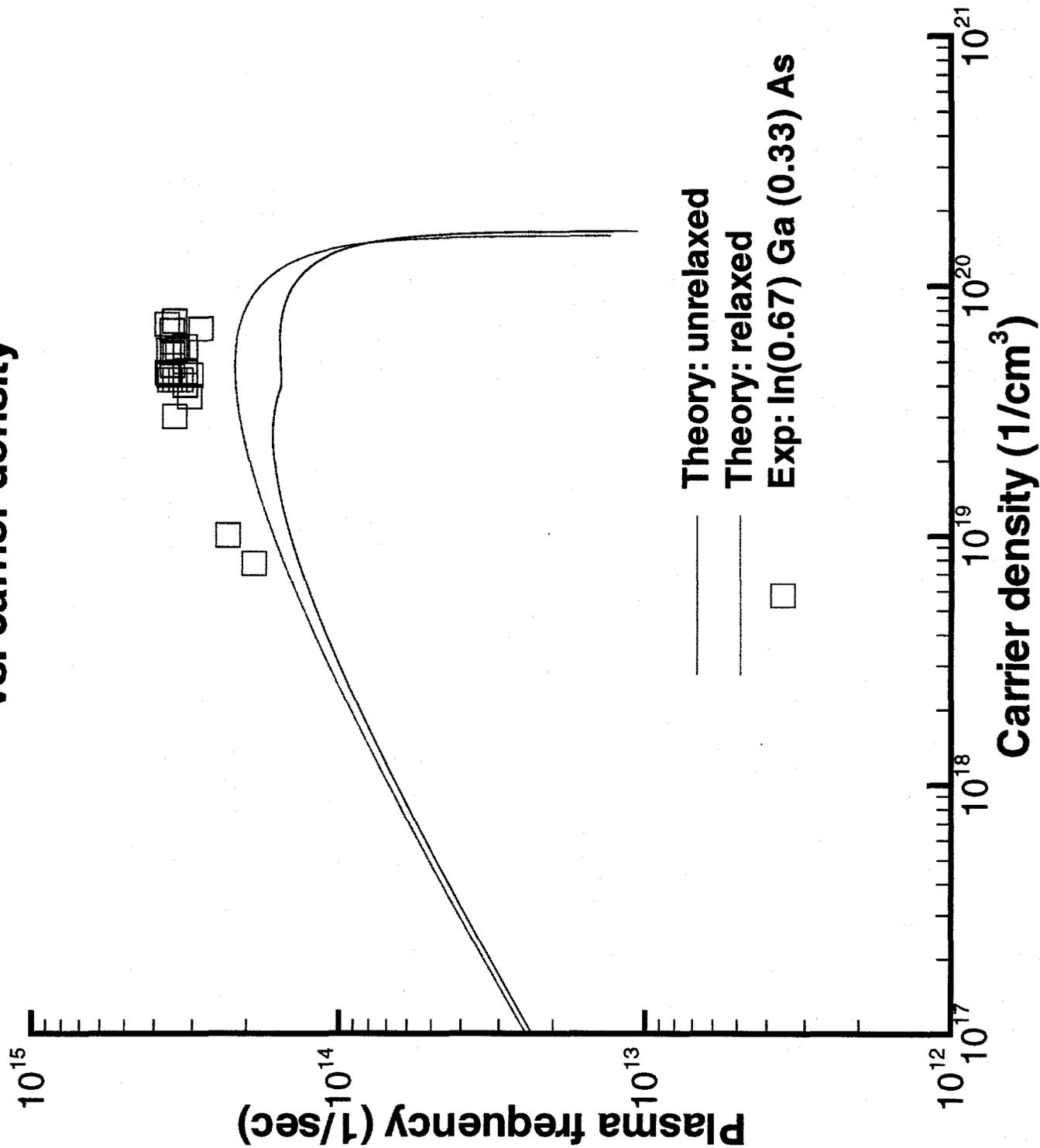


Fig. 1

# In(0.75) Ga(0.25) As: Fermi energy vs. carrier density

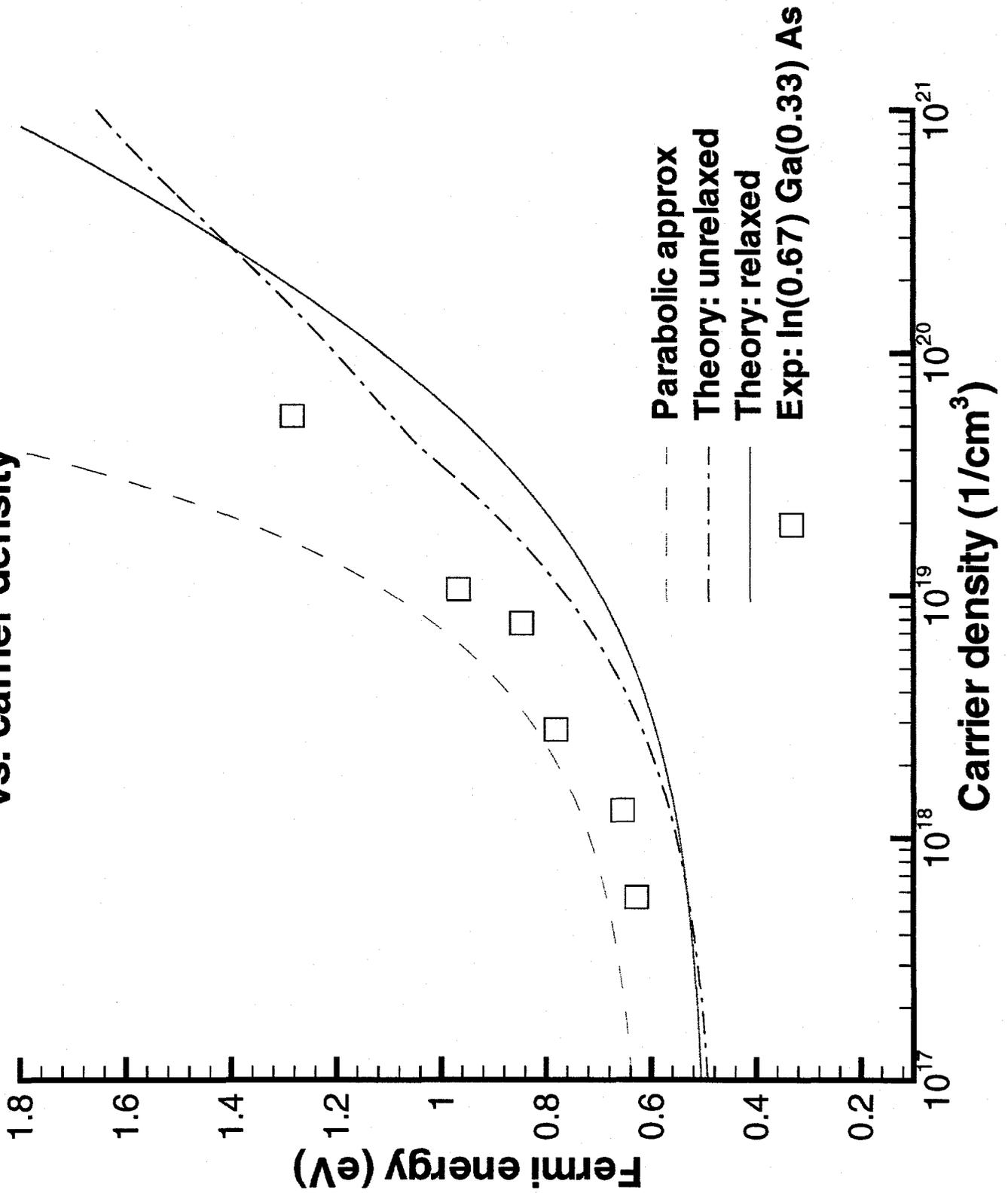


Fig. 2