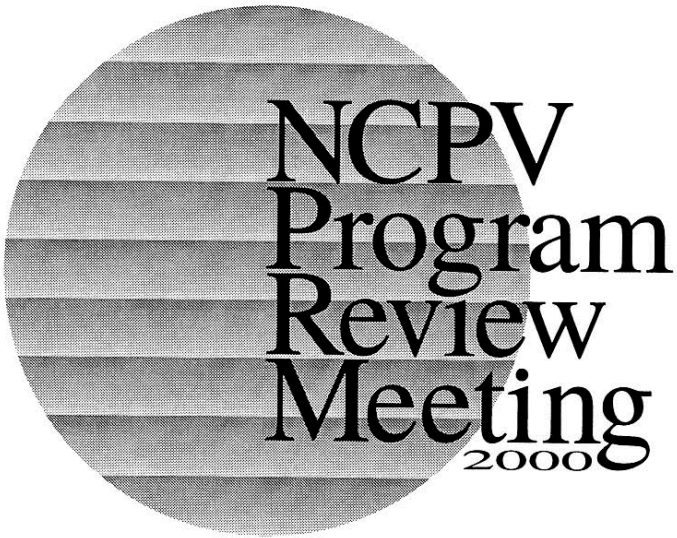
ADDENDUM TO THE PROCEEDINGS



April 16–19, 2000

Adam's Mark Hotel

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Nitrogen-induced evolution of $GaAs_{1-x}N_x$ studied by ballistic electron emission spectroscopy

V. Narayanamurti,[1] M. Kozhevnikov,[1] H.P. Xin,[2], C.W. Tu,[2] A. Mascarenhas[3] and Y. Zhang[3]

[1]Division of Engineering and Applied Sciences, Harvard University, 9 Oxford Street, Cambridge, MA 02138

[2] Electrical and Computer Engineering Department, University of California at San Diego, La Jolla, CA 92093

[3] National Renewable Energy Laboratory, 1617 Cole Boulevard, Golden, CO 80401

ABSTRACT

Giant bandgap reduction of dilute $GaAs_{1-x}N_x$ with nitrogen incorporation makes this material to be very attractive for conversion efficiency increase in multijunction, high efficiency solar cells. This paper reports on an experimental study of GaAsN band structure at low nitrogen concentrations by ballistic electron emission microscopy spectra. We present consistent results on the GaAsN conduction states evolution and a giant reduction of the Schottky barrier height as a function of the nitrogen concentration (up to x=0.021).

1. Introduction

In spite of the remarkable achievements in fabricating high-efficiency cells with III-V semiconductors, e.g. a high efficiency (>30%) monolithic GaInP/GaAs tandem cells [1], any further improvement will require incorporation of a third junction consisting of a semiconductor with a bandgap in the range of 0.95-1.1 eV. Giant bandgap reduction of dilute $GaAs_{1-x}N_x$ with nitrogen incorporation, by more than 0.4 eV at x~0.04, makes this material to be very attractive for conversion efficiency increase in multijunction, high efficiency solar cells. Despite the obvious progress in the experimental and theoretical study of GaAsN anomalies, little is known about the intrinsic electrical and optical properties of GaAsN surface and subsurface. To shed new light on the band structure we report here the first measurements of the electron transport in the conduction band of these alloys using the ballistic electron emission microscopy (BEEM) technique [2].

2. Samples and experimental approach

A 1000 Å undoped $GaAs_{1-X}N_X$ layer and 1000 Å n^+-GaAs buffer layer were grown on n^+ (001)-oriented GaAs substrates by gas source molecular beam epitaxy at 420°C [3]. A detailed analysis is presented here for the nitrogen compositions of x=0, 0.003, 0.005, 0.007, 0.012, 0.017 and 0.021. The details of the diode fabrication procedure have been published elsewhere [4]. The BEEM measurements were performed with a Surface/Interface AIVTB-4 BEEM/STM system using a Au tip. The tip-to-base voltage (V_t) was varied between 0.3 and 2.3 V to acquire the BEEM current (I_c) while keeping a constant tunneling current (I_t) of 4 nA.

3. Results

The room-temperature second derivative (SD)-BEEM spectra extracted from the experimental BEEM spectra by numerical differentiation with a 10 meV window are shown in Fig. 1. The SD-BEEM current is approximately the heterostructure transmission coefficient [5] and, therefore, allows an explicit energetic partitioning of the transport channels. Two main features (peaks) observed in the SD-BEEM spectra we associate with the Γ-like and *L*-like conduction minima in GaAsN [6]. As the nitrogen concentration increases, the low-energy threshold shifts towards lower voltages whereas the high-energy threshold shifts towards higher voltages The inset of Fig.2 shows that the relative *L*-like band contribution to the BEEM current reduces by two thirds as the nitrogen concentration increases from 0.3% to 2.1%.

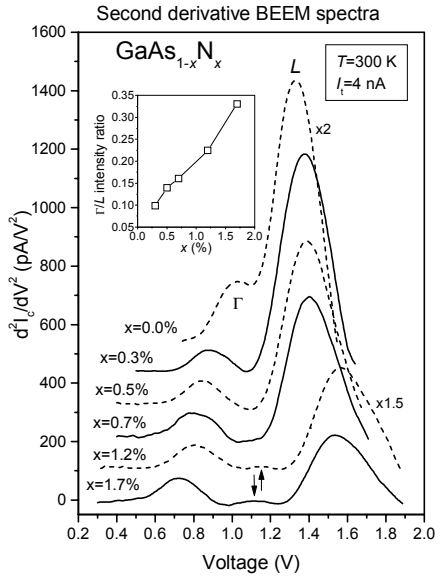

Figure 2. Room temperature SD-BEEM spectra for six different nitrogen compositions (from 0 to 0.017). For clarity, the SD-BEEM spectra are shifted along the vertical axis. The inset shows the ratio of the Γ-like peak to the *L*-like peak as a function of the nitrogen concentration.

The compositional dependencies of the thresholds observed in the SD-BEEM spectra are plotted in Fig. 2. While the Γ-like threshold decrease has a nearly linear compositional dependence up to x=2.1%, the *L*-like

threshold position increases initially at x≤1.2% and then is almost constant. The energetic separation between Γ-like and *L*-like transport channels as a function of the nitrogen composition is close to but exceeds slightly (<0.1 eV) the recently reported E_+-E_0 dependencies in optical experiments [7,8]. This difference between the *L*-like and E_+ energies above the conduction band edge is most likely due to the difference in the experimental techniques. In both the BEEM and optical techniques, the observed high-energy state is a weighted combination of the conduction states, but the BEEM weighting of the different bands is proportional to their DOS's [9], while the optical transition probability is defined by their Γ-character [8,10]. Since nitrogen substitution results in the splitting of the fourfold *L* valley into the $a_1(L_{1c})$ singlet and $t_2(L_{1c})$ triplet states [7,8] the *L*-like band in the BEEM experiments is mostly weighted on the $t_2(L_{1c})$ triplet state, and the E_+ transition is mostly weighted on the $a_1(L_{1c})$ singlet state.

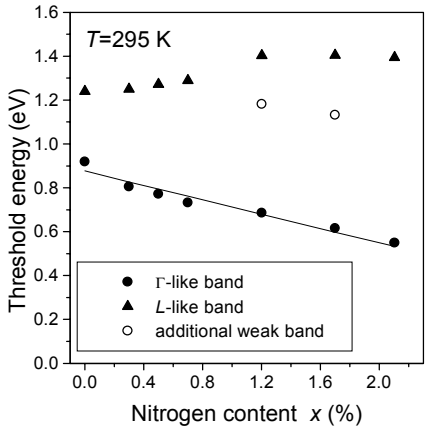

Figure 2. The compositional dependencies of the thresholds observed in the SD-BEEM spectra of $GaAs_{1-X}N_X$. The solid line is the best linear fit to the Γ-like threshold giving a slope of –16.4 eV.

The SD-BEEM spectra of two GaAsN samples, *x*=1.2 and 1.7 (see Fig. 1), reveal an additional weaker peak (indicated by the arrow), located ~0.40 eV and ~0.43 eV above the Γ-like state, respectively. This peak might represent the contribution from the $a_1(L_{1c})$ singlet state. The weaker amplitude of this peak matches the expected small DOS due to the increasing Γ-character of the $a_1(L_{1c})$ state in the alloy limit [10].

As the nitrogen concentration increases, the Au/GaAsN Schottky barrier (Γ-like threshold) decreases considerably, as shown in Fig. 2. The solid line in Fig. 2 is the best linear fit to the experimental data (with a slope of –16.4 eV). Using E_g(GaAs)=1.42 eV and E_g(GaN)=3.5 eV at room temperature, the same slope of E_g(GaAsN) would correspond to the bowing parameter of -18.9 eV. This value of the E_g bowing parameter is in a good agreement with the experimental estimates [11]. Thus we conclude that the nitrogen-induced Schottky barrier reduction accommodates most of the bandgap reduction in GaAsN. This result that is very important for device applications indicates that the effect of the nitrogen incorporation on the valence band is small.

4. Conclusions

The evolution of $GaAs_{1-X}N_X$ band structure at low nitrogen concentrations (up to *x*=0.021) was studied by BEEM. The SD-BEEM spectra of GaAsN show two main peaks, which we associate with the contribution of the Γ-like and *L*-like bands of GaAsN. As the nitrogen concentration increases, the energetic separation between these peaks increases as well, with a relative decrease of the *L*-like band contribution to the BEEM current. Another prominent effect of the nitrogen incorporation is a giant decrease of the Au/GaAsN Schottky barrier, from ~0.92 eV at *x*=0 down to ~0.55 eV at *x*=0.021. The observed Schottky barrier reduction follows approximately the bandgap reduction.

In future, we plan to extend our study to GaInAsN alloys that can be lattice matched to GaAs (Ge) by adjusting the In and N contents. It promises an additional controllable decrease of the bandgap, allowing the optimization of the solar cell efficiency.

The authors would like to thank Dr. N.A. Modine for helpful discussions. The support of the Midwest Research Institute under Department of Energy PV Program is gratefully acknowledged.

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