MONTE CARLO SIMULATION OF HIGH FIELD ELECTRON TRANSPORT IN ZnS WITH MODIFIED DENSITY OF STATES

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ABSTRACT

An ensemble Monte Carlo simulation has been developed for electrons in ZnS which includes three nonparabolic valleys in the first conduction band as well as a single nonparabolic valley in the second conduction band. The density of states for the first band was modeled phenomenologically to resemble the density of states obtained by numerical pseudopotential calculations. This density of states was used only in the calculation of the scattering probabilities and no attempt was made to modify the conductivity effective mass. The scattering probabilities included in the simulation are those due to ionized impurities, acoustic phonons, polar optical phonons, intervalley phonons, and impact ionization. It is found that the inclusion of the second band and modification of the density of states effective mass has a dramatic effect on the energy distribution, especially at fields above 1MV/cm. When the field exceeds 1MV/cm, the distribution begins to show a secondary peak associated with the second band that is not found in previous investigations. At lower fields, the second band contributes a high energy tail but does not alter the peak of the energy distribution noticeably. The importance of introducing the second band is that, because the width of the first band is less than the band gap, it is believed that nearly all band to band impact ionization is due to electrons in the second conduction band. This has specific relevance in the operation of ZnS AC thin-film electroluminescent devices.

I. INTRODUCTION

An understanding of the high field transport properties of electrons in ZnS is essential for the design and operation of many AC thin film electroluminescent (ACTFEL) devices. These devices operate at fields ranging from 0.5 MV/cm to 2.0 MV/cm and rely on highly energetic (hot) electrons for both the excitation of the activator as well as the for the process of carrier multiplication via band to band impact ionization. At present very few attempts have been made to investigate the behavior of this material in the high field regime. Previous studies, [1,2] have indicated that the electron distribution in ZnS is relatively cool with the high energy tail of the distribution ending at less than 4.0 eV even for fields up to 2.0 MV/cm. While Brennan [1] included the full structure of both the first and second conduction band, it is not clear what his results imply in terms of impact ionization in ZnS, since his work is mainly a comparison between ZnS and ZnSe, and results for fields in excess of 1.0 MV/cm were not reported. Bhattacharyya et al [2] used a model that included only the first conduction band in a infinite nonparabolic three valley model. Their model is not consistent with the band structure or density of states of ZnS at these high fields because the electrons were found to have energies exceeding the energy depth of the first conduction band. Müller et al [3] have used a single parabolic valley in the first conduction band. This again is unrealistic at these fields and this model leads to an unstable distribution with ballistic, loss free transport.

One method of including higher bands is to use a method suggested by Brunetti et al [4]. This model uses a band structure so chosen as to give the density of states function a good fit with experimental and theoretical determinations. Our model consists of three valleys in the first conduction band and one valley in the second conduction band with the valley parameters of the second conduction band chosen so as to give a good fit with the density of states as determined by numerical pseudopotential calculations [5,6]. Typically, when an effective mass approach is taken, no steps are taken to insure that the density of states of the first conduction band begins to decrease when the top of the band is approached. We have taken the density of states effective mass to be energy dependant so that the density of states does not extend infinitely. This method affects the scattering rate only by not allowing transitions to states at energies within valleys where no states exist. We have also added a second conduction band, with a single valley X2, that has valley parameters similar to the X valley in the first band. The energy of the X2 valley bottom was taken to be 2.2 eV above the bottom of the gamma valley. The conductivity effective mass was not altered

and is energy independent. Other than this change, we have used the same scattering rate calculations as Bhattacharyya et al [7,8]. Since the ACTFEL devices that are of interest to us are polycrystalline, the electric field is not taken in any specific crystal direction.

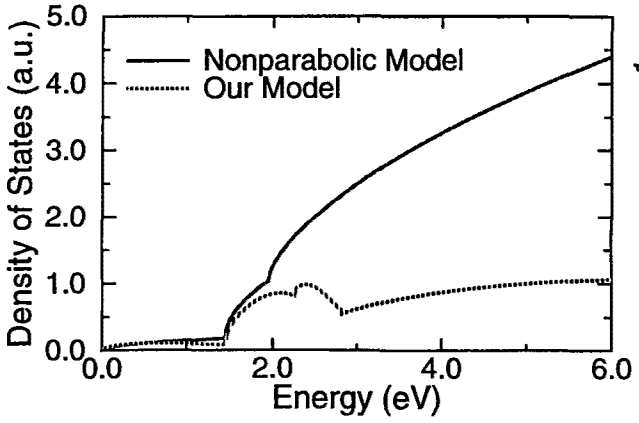

Fig. 1. The electron density of states in the conduction band of ZnS in both the simple infinite valley nonparabolic model, and our approach.

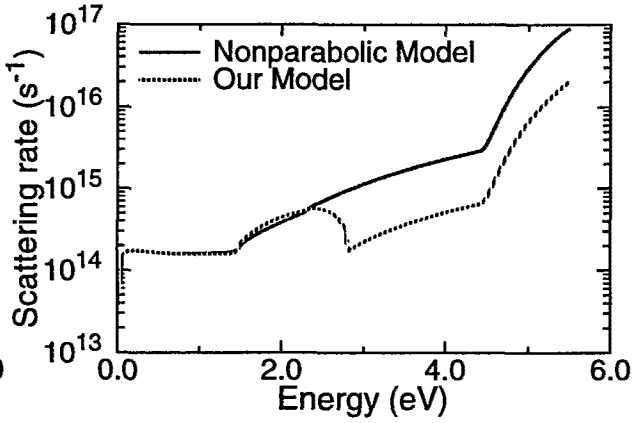

Fig. 2. The electron total scattering rate in the gamma valley for the simple infinite valley nonparabolic model, and our approach.

II. RESULTS

Fig 1. shows the density of states of the conduction band in our approximation as well as the simple, nonparabolic model used by Bhattacharyya. Our approximation more closely resembles the density of states computed by pseudopotential model than the simple infinite nonparabolic valleys yet it also requires much less computational time than that of Brennan's full band approach. Fig 2 shows the total scattering rate for the gamma valley as a function of energy. Because of the way that the density of states mass is defined, the scattering rates represent a sort of convolution of the scattering rate given by Bhattacharyya and the theoretical density of states. The simple infinite valley approach tends to overestimate the scattering rates at high energies, resulting in cooler distributions. For the gamma valley, polar optical scattering dominates at low energies. At 1.5 eV intervalley scattering to first conduction band valleys begins to dominate. When the electrons have acquired enough energy to scatter to the second band this process begins to dominate until the threshold for impact ionization is reached. Impact ionization is the dominant scattering mechanism for electrons in any valley once the total energy exceeds the threshold energy for impact ionization. Acoustic scattering is more important at high energies while ionized impurity scattering is more important at low energies but neither of these scattering mechanisms are ever dominant at any energy. For all of the upper valleys, intervalley scattering is the dominant scattering mechanism at all energies until the onset of impact ionization.

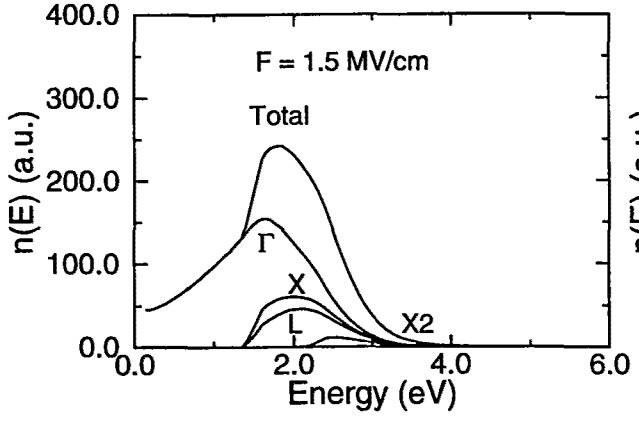

Fig. 3. Four valley, two band electron energy distribution for ZnS at 1.5 MV/cm in the simple infinite valley nonparabolic model.

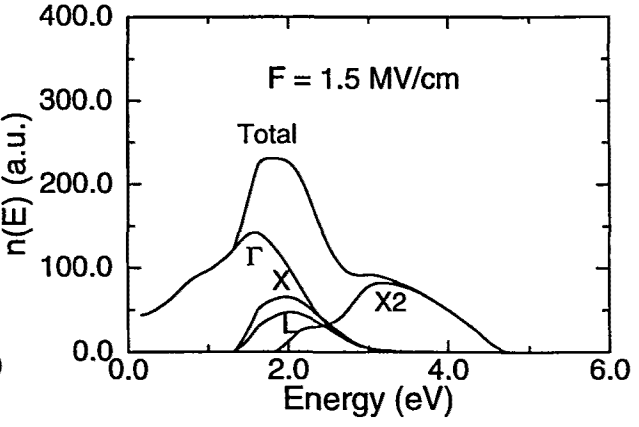

Fig. 4. Four valley, two band electron energy distribution for ZnS at 1.5 MV/cm in our model

Figs. 3 and 4 show the steady state electron energy distribution n(E) plotted as a function of energy for each valley in the first two conduction bands for an electric field of 1.5 MV/cm which is a typical field for an ACTFEL device [9]. Fig. 3 shows the distribution as it is calculated in the infinite valley approach and showing the cool distribution, while Fig. 4 shows the same distribution calculated in our approach showing an enhanced tail which extends past the threshold for impact ionization. At low fields, the total distribution is not that much different from the results of Bhattacharyya et al, the tail of the distribution begins to slope off at less than 4.0 eV. For higher fields, the results are quite new. We predict an enhanced tail and the formation of a secondary peak in the energy distribution at about 3.3 eV. The inclusion of the second conduction band, and lowering of the scattering rates allows the energy distribution to become hotter.

Impact ionization rates were calculated at several different fields, and Fig. 5 shows the impact ionization rate vs. the inverse field plotted on a semi-log scale to show the linear dependence. The data points are obtained from the simulation while the solid line is the impact ionization field dependence we have used to model ZnS ACTFEL devices as shown in Fig. 6. The impact ionization rate dependance supports the work of Shockley [10] which gives an ionization rate that depends on the field as

$$\alpha \sim \exp\left(\frac{B}{|E|}\right)$$

where E is the electric field strength and B is a constant. The results of the simulation determine B to be 3.95×10^6 V/cm

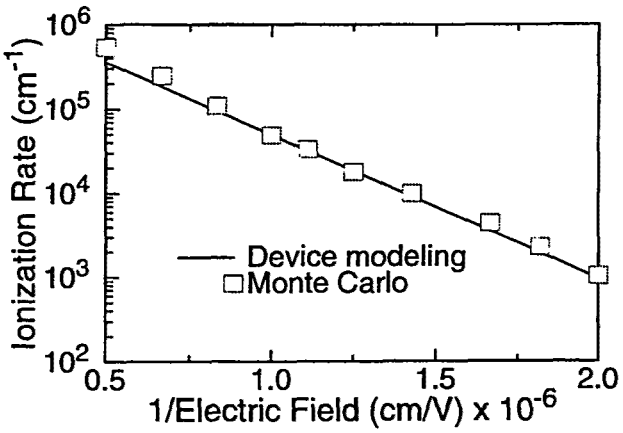

Fig. 5. Impact ionization rate for electrons in ZnS as a function of the inverse applied electric field.

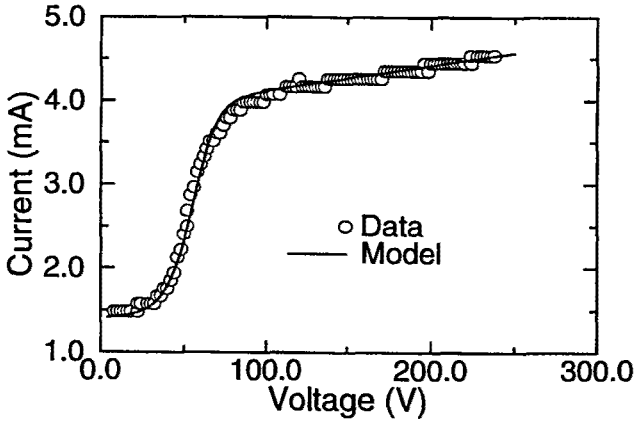

Fig. 6. I-V curve for a ZnS ACTFEL device showing both experimental data and device modeling based on the impact ionization rate derived from the simulation.

III. DISCUSSION

The results of the simulation clearly indicate that because of the high field heating of the electrons, the second conduction band can not be ignored. This simulation was not meant to include the full band structure in the calculations but rather a first approximation to the behavior of the electrons when a second conduction band is included. Just blindly adding a second band will not have much effect on the distribution though, since the infinitely extending valleys lead to an overestimation of the density of state in the first band which in turn leads to unrealistically high intervalley transfer into the first band. At low fields, the results of our simulation agree qualitatively with the results of Bhattacharyya et al [2] and this is evidence of the validity of the approximation in the limit of low fields. The simulation suggests that the second conduction band is sufficiently populated to support impact ionization rates that are high enough to drive the current voltage characteristics of a typical ZnS ACTFEL device. Previously it was thought [1,2,11] that impact ionization was at best a secondary source of electrons with the most important contributions coming from the tunneling of electrons from the interface states. Our simulation suggests that impact ionization is probably the dominant source of the electrons involved in the gain behavior of the devices. The work of Müller et al [3] and Mach [12] was done with a single parabolic valley and ballistic electron transport was reported. In our model, the single valley in the second conduction band acts in a similar manner, and if impact ionization is not included in the simulation, ballistic electron transport is also encountered

with an unstable energy distribution. We believe that the first conduction band supports a stable electron distribution due to the high scattering rates that intervalley scattering introduces. In the second conduction band on the other hand, the electrons in the X2 valley will impact ionize before they have enough energy to scatter to other second band valleys. Only electrons with low kinetic energy can scatter back into the first conduction band because there are no states available at higher energies in the first conduction band for them to transfer to. The first conduction band is still responsible for the supply of electrons that impact excite the luminescent centers since most of these have excitation energies of 2-3 eVs. At high enough fields however, the simulation suggests that there will be a second peak in the distribution. The secondary peak is in the second band and is located around 3.3 eV. This peak could be utilized to excite other luminescent centers if a proper dopant is found.

IV. CONCLUSIONS

Monte Carlo simulation of electrons in ZnS indicates the importance of the inclusion of the second conduction band. The electron population of the second band has a significant impact on the electron energy distribution as well as the impact ionization rate. Because the density of states of the first conduction band was limited so that electrons were not able to scatter into states with energy greater that the top of the band, there is a reduction in the scattering rate in the second band at about 3.0 eV. This reduction of scattering rates leads to a second peak in the conduction band which begins to show up for fields above 1.0 MV/cm. Results show that impact ionization is a reasonable candidate for a source of carrier multiplication in ZnS ACTFEL devices.

ACKNOWLEGEMENTS

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