

Monte Carlo Simulations of High Field Transport in Electroluminescent Devices

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High field transport in phosphor materials is an essential element of thin film electroluminescent device performance. Due to the high accelerating fields in these structures (1-3 MV/cm), a complete description of transport under high field conditions utilizing information on the full band structure of the material is critical to understand the light emission process due to impact excitation of luminescent impurities. Here we investigate the role of band structure for ZnS, GaN, and SrS based on empirical pseudopotential calculations to study its effect on the high field energy distribution of conduction band electrons.

Keywords: High field transport, Monte Carlo method, ZnS, GaN, SrS

INTRODUCTION

Over the past ten years, thin film electroluminescent (TFEL) devices have become an important technology for flat-panel display applications [1]. A TFEL device essentially consists of a thin layer of a phosphor material sandwiched between two insulating layers which are contacted by electrodes. Wide band gap semiconductors such as ZnS and SrS heavily doped with a luminescent impurity are currently the most important commercial phosphor materials. Above a critical potential applied to the electrodes of a ZnS based TFEL

device, electrons are injected into the phosphor layer from deep trap states at the phosphor-insulator interface. For sufficiently high phosphor fields, the electrons gain kinetic energy large enough to initiate impact excitation of the luminescent impurities such as Mn^{2+} to excited levels. Visible light is emitted when the impurities return back to the ground state. SrS doped with Ce^{3+} has recently demonstrated good efficiency as a blue phosphor material in TFEL applications, which is critical to realizing full color (RGB) displays. Typically, the turn on fields are higher than those of ZnS devices, which may be

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associated with the high field transport properties of this material. GaN is another wide band gap material with a similar band structure to ZnS, which is currently of interest for high temperature electronics and visible optical sources. However, the efficiency of GaN phosphors in TFEL devices is poor, which is not understood at this time.

The purpose of the present work is to investigate the relative high field transport properties of zincblende-type ZnS and GaN as well as SrS based on band structure features by Monte Carlo methods. In order to better understand the operation of electroluminescent devices, it is critical to know to which extent the TFEL performance is determined by the transport in the phosphor material.

MONTE CARLO MODEL

The ensemble Monte Carlo code presented in this paper includes the full band structure information of the phosphor material and all the pertinent scattering mechanisms to solve the semi-classical Boltzmann transport equation under high field conditions. Our approach basically follows the model developed by the Illinois group, which is described in detail elsewhere [2].

The standard empirical pseudopotential method (EPM) is employed to obtain the band structure for ZnS, GaN, and SrS. In the case of ZnS, we have extended the local EPM calculation reported by Walter and Cohen [3] and have included also nonlocal corrections in the pseudopotential [4]. The new nonlocal parameter set was determined by comparing to optical data for this material [5]. For GaN, the local EPM parameters published by Fan *et al.* [6] have been used in the calculation. Their form factors were obtained by adjusting the band structure results along directions of high symmetry to results based on *ab initio* techniques and to experimental data for band gaps and effective masses. In the case of SrS, we have derived a nonlocal EPM band structure, since a reliable EPM calculation is not yet available in the

literature. As a starting point, we have utilized the atomic pseudopotentials for Sr and S, and combined them using the method suggested by Harrison [7] to give a first estimate of the band structure. The resulting energy dispersion gives a direct gap at the Γ point. Relying on various first principles calculations [8,9], SrS is believed to be an indirect semiconductor with an indirect gap close to 4 eV occurring at the X point. We have therefore added nonlocal corrections to the local form factors to accomplish the transition to an indirect band gap material. Other than the energy band gaps at the X and Γ point [10], we are aware of no experimental band structure data for this material. Thus, the accuracy of the calculated energy dispersion is at present unknown. Furthermore, the number of 181 plane wave states employed in the expansion of the crystal wave functions might not be large enough in the case of SrS to ensure convergence of the energy levels due to its pronounced ionic character [11]. Figure 1 shows a comparison of the DOS for ZnS, GaN, and SrS. As can be seen, the DOS for SrS is dramatically larger than the DOS for ZnS and GaN.

The scattering rates for various mechanisms in the semiconductor material are calculated based on first-order time dependent perturbation theory. For energies below higher valley minima, we use a

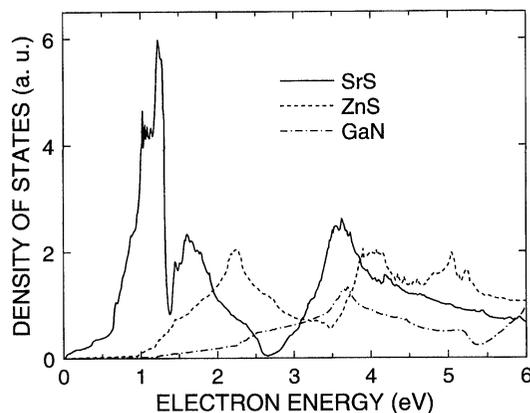


FIGURE 1 Comparison of the density of states for ZnS, GaN and SrS.

nonparabolic band model to compute the scattering rates in the lowest lying valley [12]. The effective mass and nonparabolicity parameter of the valley entering into the scattering rates were extracted directly from the EPM calculation of the band structure. The scattering mechanisms taken into account include scattering due to polar optical phonons, acoustic and optical phonons via the deformation potential interaction and ionized impurities. At energies above higher valley thresholds, electron scattering is dominated by the optical deformation potential mechanism. To lowest order, this mechanism is isotropic in nature and depends only on the density of final states. Therefore, the DOS shown in Figure 1 is used directly to determine the scattering rate at high energy. Reported measurements of the optical deformation potentials for inter- and intravalley scattering in ZnS, GaN, or SrS do not exist to our knowledge. For this reason, we treat the deformation potentials as adjustable parameters by fitting to carrier multiplication data, when available.

An inevitable scattering mechanism for the stabilization of the electron distribution function at high electric fields is band-to-band impact ionization of electron-hole pairs by energetic electrons. Here, we use an energy dependent impact ionization rate averaged over all directions in wave vector space, calculated numerically from the full band structure of the wide band gap semiconductor and well represented by a power law [5], [13]. In our Monte Carlo simulations, this fit formula is incorporated into the collision term of the Boltzmann equation.

RESULTS AND DISCUSSION

In the ensemble Monte Carlo simulations presented here, we have included the first four conduction bands of each semiconductor studied. The full band structure is represented using 916 points in the irreducible wedge of the first Brillouin zone. Typically, an ensemble of 96,000 particles is followed in order to achieve sufficient accuracy in

simulating rare events such as impact ionization and impact excitation.

Although systematic experimental studies of high field transport in wide band gap semiconductors such as ZnS, GaN, or SrS are currently not available, information regarding the high field distribution may be indirectly deduced from measurement of carrier multiplication due to band-to-band impact ionization. Such measurements were performed for ZnS by Thompson and Allen [14]. We have used a set of two optical deformation potentials, one characterizing the lowest conduction band, and the other characterizing the upper bands, to bring our simulated results for the impact ionization coefficient versus field into agreement with Thompson and Allen's data. The details of this choice of proper deformation potentials have been discussed in Reference [5]. We are not aware of any carrier multiplication measurement for GaN and SrS. Owing to this lack of information, values of deformation potentials identical to those in ZnS have been assumed in the Monte Carlo simulations. By assuming the same deformation potentials for each material, we are able to make a comparison of the high field transport properties of these three materials based on the band structure itself.

Figure 2 shows the simulated steady-state particle distribution (i.e., the number of particles in a given energy range) in ZnS, GaN, and SrS for an electric field of 2 MV/cm at 300 K. For Mn^{2+} impurities in ZnS with an excitation threshold energy of approximately 2.1 eV, the comparison of ZnS to GaN indicates that there are more electrons above the impact excitation threshold due to the lower DOS for GaN, and significantly fewer electrons in the case of SrS due to its high DOS. The secondary peak in the distribution for ZnS at about 4 eV is directly related to the minimum in the DOS shown in Figure 1. Since a lower DOS translates to a reduced optical deformation potential scattering rate, the trends in the DOS are clearly reflected in the simulated high field distributions, provided that the assumption of identical deformation potentials is not too

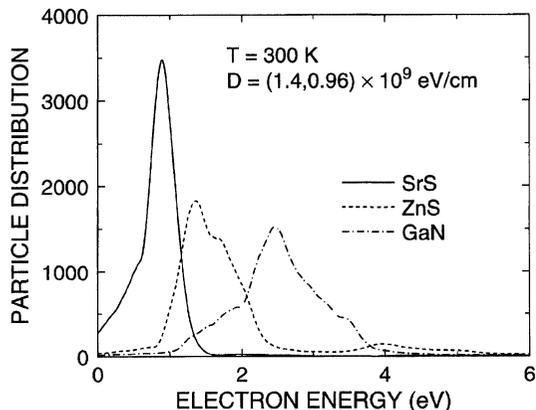


FIGURE 2 Simulated particle distribution in ZnS, GaN and SrS for an electric field of 2 MV/cm at a lattice temperature of 300 K assuming identical deformation potentials.

unrealistic. Our results seem to suggest that the high field properties of GaN would be superior to those of ZnS in TFEL device operation, and that SrS has less favorable transport properties. High field transport in SrS might improve at higher fields because of the tendency towards reduced DOS with increasing kinetic energy, as can be seen from Figure 1. The uncertainty with regard to the operation of a SrS device is how much of a role is played by space charge and how large is the cathode field under device operation. There is experimental evidence that the cathode field may be significantly larger than the measured, average field due to large amounts of space charge [15]. These effects have been ignored in the present work.

Figure 3 shows the impact excitation yield and impact ionization yield for electrons traversing a ZnS layer of 0.5 μm thickness for various electric fields. The impact excitation rate of Mn luminescent impurities in ZnS used in the Monte Carlo simulations has been calculated from the transition rate derived by Bringuier [16] based on the exchange scattering process. For Mn impurities embedded in ZnS, exchange scattering is known to be the dominant excitation path. We have performed the high field simulations for two

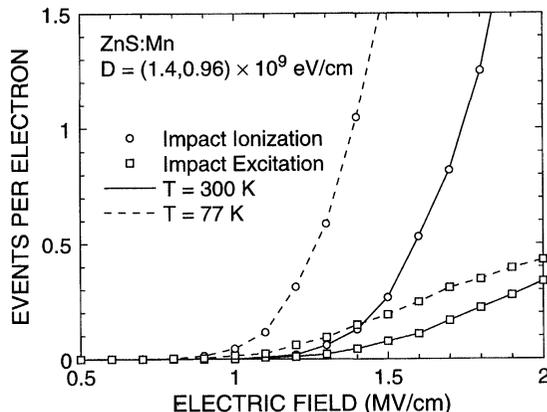


FIGURE 3 Simulated impact ionization and impact excitation yields for various electric fields in a ZnS layer of 0.5 μm thickness doped with Mn. Shown are the results for two different lattice temperatures.

different lattice temperatures: $T=300\text{ K}$ and $T=77\text{ K}$. For both temperatures, the impact ionization yield is larger than the corresponding excitation yield for a density of 10^{20} cm^{-3} Mn atoms. The comparison reveals that impact excitation as well as impact ionization increases with decreasing lattice temperature since the scattering of electrons due to phonons is reduced. At the lower temperature, the electron system reaches a higher average energy in the steady state so that more electrons are capable to impact excite luminescent impurities or to generate electron-hole pairs by band-to-band impact ionization.

CONCLUSIONS

We have simulated high field transport in ZnS, GaN, and SrS including the full band structure of these materials in a Monte Carlo simulation. The simulated steady-state distributions of electrons at typical phosphor fields reveal good transport properties of ZnS and GaN. High field transport in SrS appears to be less favorable, although space charge effects might be very important. We find good agreement in the expected trends of the impact excitation yield with temperature in ZnS

based TFEL devices. The optical deformation potential is the greatest uncertainty in the present Monte Carlo model, which suggests further investigation of the electron-phonon coupling in phosphor materials is needed in order to understand their high field behavior.

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Manfred Dür received the M.S. and Ph.D. degrees in physics from the University of Innsbruck, Austria, in 1990 and 1995, respectively. He is currently working as a Faculty Research Associate at the Department of Electrical Engineering at Arizona State University. His research interests include high field transport in electroluminescent materials and relaxation processes in quantum confined systems.

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Martin Reigrotzki studied physics at the Swiss Federal Institute of Technology in Zürich where he received his diploma in theoretical physics in 1994. Since 1994, he is working as a Ph.D. student with Professor Redmer at the University of Rostock on high field electron transport in semiconductors.

Ronald Redmer received his Ph.D. in theoretical physics in 1986 and was awarded the habilitation grade in 1991, both from the University of Rostock. He is now Professor for theoretical physics at the University of Rostock. His primary interests concern the high field electron transport in semiconductors and the properties of dense plasmas and expanded fluids.



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