The diffusivity– mobility ratio in heavily doped nonlinear optical, optoelectronic and related materials

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ABSTRACT

We study the diffusivity–mobility ratio (DMR) in heavily doped nonlinear compounds forming band tails on the basis of a newly formulated electron dispersion law and III–V, ternary and quaternary materials form a special case of our generalized analysis. The complex nature of the energy spectrum and creation of a new forbidden zone is the consequence of anisotropic energy band constants and the interaction of the impurity atoms in the tails with spin–orbit splitting of valence bands for the other compounds. Analytically, the presence of non-removable poles in the dispersion relation of the undoped material creates the complex energy spectrum for the corresponding heavily doped sample. The DMR for the heavily doped II–VI, IV–VI and stressed materials has been studied. It has been found taking n-type $CdGeAs_2$, Cd_3As_2, InAs, InSb, $Hg_{1-x}Cd_xTe$, $In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP, CdS, PbTe, PbSnTe, $Pb_{1-x}Sn_xSe$ and stressed InSb as examples that the DMR increases with the increasing electron concentration with different numerical values and the nature of variations are totally band structure dependent. An experimental method of determining the DMR in heavily doped materials for arbitrary dispersion relations together with three applications in the area of material science in general has been suggested.

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1. Introduction

It is well known that the diffusivity–mobility ratio (DMR) occupies a central position in the whole field of nanoscience and technology since the diffusion constant (a quantity very useful for device analysis whose exact experimental determination is rather difficult) can be derived from this ratio by knowing the experimental values of the mobility. In addition, it is more accurate than any of the individual relations for the diffusivity or the mobility which are two widely used quantities of carrier transport of nano-devices. The classical value of the DMR is equal to $k_BT/|e|$ (k_B, T and $|e|$ are the Boltzmann constant, temperature and the magnitude of the carrier charge respectively) and is well-known in the literature as Einstein relation [1]. In this conventional form it appears that the DMR increases linearly with T and is independent of electron concentration. This relation is valid for both electrons and holes. Besides, the relation holds only under the condition of non-degenerate carrier concentration, although

its validity has been suggested erroneously for degenerate materials [2]. It is well known that the performance of the electron devices at the device terminals and the speed of operation of modern switching transistors are significantly influenced by the degree of carrier degeneracy present in these devices [3]. The simplest way of analyzing such devices taking into account the degeneracy of the bands is to use the appropriate Einstein relation to express the performance at the device terminals and the switching speed in terms of the carrier density [4]. In this context, we wish to note that the connection of the DMR with the velocity autocorrelation function, its relation with the screening length [5] and the noise power (under non-degenerate condition) [6,7] has also been studied.

It is well known from the fundamental works of Landsberg [8] that the Einstein relation in degenerate materials is essentially determined by the energy band structures. It has, therefore, different values in different materials and varies with electron concentration, with the magnitude of the reciprocal quantizing magnetic field under magnetic quantization, with quantizing electric field as in inversion layers, and with the supperlattice period as in quantum confined superlattices of small gap semiconductors with graded interfaces having various carrier

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energy spectra. The nature of these variations has been investigated by Ghatak and co-workers [9,10] and few others [11–15]. Some of the significant features which have emerged from these studies are:

(a) The ratio increases monotonically with electron concentration in bulk semiconductors.
(b) The nature of the variations is significantly affected by the band non-parabolicity.
(c) The ratio increases with the magnitude of quantizing electric field in inversion layers.
(d) The ratio oscillates with the inverse quantizing magnetic field under magnetic quantzation due to the SdH effect.
(e) The ratio exhibits composite oscillations with the superlattice period in various types superlattices having different dispersion relations.

The above characteristics are considered as theoretical predictions and no experimental results are available, to the knowledge of the authors, in support of the predictions for the heavily doped degenerate materials forming band tails. The lack of experimental results emanate from the difficulty in the measurement of the diffusion constant D for degenerate materials under the condition of heavy doping. It appears from the literature that the DMR in heavily doped nonlinear optical, ternary, quaternary, II–VI and IV–VI and stressed materials has yet to be investigated in details by considering all types of anisotropies within the framework of $\mathbf{k} \cdot \mathbf{p}$ formalism.

It is well known that the band tails are being formed in the forbidden zone of heavily doped semiconductors and can be explained by the overlapping of the impurity band with the conduction and valence bands [16]. Kane [17] and Bonch Bruevich [18] have independently derived the theory of band tailing for semiconductors having unperturbed parabolic energy bands. Kane's model [17] was used to explain the experimental results on tunneling [19] and the optical absorption edges [20,21] in this context. Halperin and Lax [22] developed a model for band tailing applicable only to the deep tailing states. Although Kane's concept is often used in the literature for the investigation of band tailing [23,24], it may be noted that this model [17,25] suffers from serious assumptions in the sense that the local impurity potential is assumed to be small and slowly varying in space coordinates [24]. In this respect, the local impurity potential may be assumed to be a constant. In order to avoid these approximations, we have developed in this paper, the electron energy spectra for heavily doped semiconductors for studying the DMR based on the concept of the variation of the kinetic energy [16,24] of the electron with the local point in space coordinates. This kinetic energy is then averaged over the entire region of variation using a Gaussian type potential energy. On the basis of the E–k dispersion relation, we have obtained the electron statistics for different heavily doped materials for the purpose of numerical computation of the respective DMRs. In a heavily doped semiconductors, each impurity atom is surrounded by the electrons, assuming a regular distribution of atoms, and it is screened independently [11,23,25]. The interaction energy between electrons and impurities is known as the impurity screening potential. This energy is determined by the inter-impurity distance and the screening radius, which is known as the screening length. The screening radius grows with the electron concentration and the effective mass. Furthermore, these entities are important for heavily doped materials in characterizing the semiconductor properties [26–28] and the devices [23,29]. The works on Fermi energy and the screening length in an n-type GaAs have already been initiated in the literature [30–32] based on Kane's model. Incidentally, the

limitations of Kane's model [24], as mentioned above, are also present in their studies.

At this point, it may be noted that many band tail models are proposed using the Gaussian distribution of the impurity potential variation [17,24]. In this paper, we have used the Gaussian band tails to obtain the exact E–k dispersion relations for heavily doped nonlinear optical, III–V, II–VI, IV–VI and stressed Kane type compounds. Our method is not at all related with the density-of-states (DOS) technique as used in the aforementioned works. It may be noted that from the electron energy spectrum, one can obtain the density-of-states but the DOS technique, as used in the literature cannot provide the E–k dispersion relation. Therefore, our study is more fundamental than those in the existing literature, because the Boltzmann transport equation, which controls the study of the charge transport properties of the semiconductor devices, can be solved if and only if the E–k dispersion relation is known. We wish to note that the Gaussian function for the impurity potential distribution has been used by many authors. It has been widely used since 1963 when Kane first proposed it. We will also use the Gaussian distribution for the present study.

In Section 2.1 of the theoretical background, the Einstein relation in heavily doped nonlinear optical materials has been investigated on the basis of the generalized dispersion relation, considering the anisotropies of the effective electron masses and the spin–orbit splitting parameters together with the proper inclusion of crystal-field splitting constant in the Hamiltonian, which are important physical characteristics of such materials. It may be noted that the nonlinear optical materials are also called as nonlinear optical compounds due to their nonlinear optical crystal structure [33]. These materials are being increasingly used in light emitting diodes, Hall pickups and thermal detectors [34–36]. Rowe and Shay [37] have demonstrated that the quasi-cubic model [38] can be used to explain the observed splitting and symmetry properties of the conduction and valence bands at the zone center of $\mathbf{k}$-space of the aforementioned compounds. The s-like conduction band is singly degenerate and the p-like valence bands are triply degenerate. The later splits into three sub-bands, because, of the spin–orbit and the crystal-field interactions. The large contribution of the crystal-field splitting occurs from the non-cubic potential [39]. The experimental data on the absorption constants [40], the effective mass [41] and the optical third-order susceptibility [42] have produced strong evidence that the conduction band in the same compound corresponds to a single ellipsoid of revolution at the zone center in $\mathbf{k}$ space. Incorporating the crystal potential to the Hamiltonian, Bodnar [43] proposed a dispersion relation for the conduction electrons in the same compound by using the assumption of an isotropic spin–orbit splitting constant although the anisotropies of the band constants are important physical features of nonlinear optical materials.

In this context, it may be noted that the III–V materials are being increasingly used in integrated optoelectronics [44], passive filter devices [45], distributed feedback lasers and Bragg reflectors [46]. Besides, we shall use n-$Hg_{1-x}Cd_xTe$ and n-$In_{1-x}Ga_xAs_yP_{1-y}$ lattice matched to InP as examples of ternary and quaternary compounds respectively. n-$Hg_{1-x}Cd_xTe$ is a classic narrow-gap compound and is an important optoelectronic material because its band gap can be varied to cover a spectral range from $0.8\,\mu m$ to over $30\,\mu m$ by adjusting the alloy composition [47]. The n-$Hg_{1-x}Cd_xTe$ finds extensive application in infrared detector materials [48] and photovoltaic detector arrays [49] in the 8–$12\,\mu m$ wave bands. The above uses have spurred an $Hg_{1-x}Cd_xTe$ technology for the production of high mobility single crystals, with specially prepared surface layers and the same material is ideally suitable for narrow sub-band physics because the relevant