

Strong non-Arrhenius temperature dependence of the resistivity in the regime of traditional band transport

C. Michel,^{a)} S. D. Baranovskii, P. J. Klar, and P. Thomas

Department of Physics and Material Sciences Center, Philipps-University, Renthof 5, 35032 Marburg, Germany

B. Goldlücke

MPI for Computer Science, Stuhlsatzenhausweg 85, 66123 Saarbrücken, Germany

(Received 6 June 2006; accepted 24 July 2006; published online 13 September 2006)

When a strong, though non-Arrhenius temperature dependence of electrical resistivity is observed, one usually concludes that the underlying mechanism is variable-range hopping. Unexpectedly, such observations are also made for many semiconductor systems at elevated temperatures, where a variable-range hopping mechanism seems unlikely. A satisfactory explanation for this observation is still lacking up to now. The authors demonstrate that a non-Arrhenius resistivity behavior may also arise in a band transport picture by thermal activation of charge carriers from a reservoir into the transport-carrying band states, provided the energy distribution of reservoir states is sufficiently broadened or the density of band states exhibits tails. © 2006 American Institute of Physics. [DOI: 10.1063/1.2348771]

In studies of transport properties of solid-state materials researchers usually devote particular attention to the temperature dependence of electrical resistivity, since this dependence is indicative for the underlying transport mechanism. Usually the direct current resistivity in doped semiconductors can be described by an Arrhenius temperature dependence, $\rho = \rho_0 \exp(\Delta/kT)$, where ρ_0 is a preexponential factor, Δ is the activation energy, and k is the Boltzmann constant. At high temperatures the so-called intrinsic resistivity is provided by thermal activation of charge carriers over the band gap and the activation energy Δ is related to the band gap energy E_g : $\Delta \approx E_g/2$. With decreasing temperature the so-called impurity resistivity mechanism takes over according to which charge carriers in the band are supplied by thermal activation from impurity atoms (donors or acceptors). The activation energy Δ in this transport mode is related to the depth of electronic levels on impurities with respect to the band edge (conduction band for donors and valence band for acceptors).¹ At even smaller temperatures the so-called hopping transport mechanism comes into play, in which carrier transport does no longer take place via band states, but instead is provided by tunneling (hopping) of charge carriers between the impurity atoms. In the latter case, the activation energy Δ is usually determined by the width of the energy distribution of charge carriers on impurity atoms. Detailed description of hopping conduction along with quantitative calculations of the activation energy Δ for this regime can be found in Ref. 2. At extremely low temperatures electrical conduction is provided by the so-called variable-range hopping (VRH). In this transport regime the Arrhenius law for $\rho(T)$ is not valid anymore. The temperature dependence of the resistivity in the VRH has the form $\rho = \rho_0 \exp[(\Delta/kT)^\beta]$, where β is determined by the shape of energy-dependent distribution of impurity (DOI) atoms. For an energy-independent DOI $\beta = 1/4$, while for the parabolic Coulomb gap in the DOI $\beta = 1/2$.²

Surprisingly, there are many experimental results of typical semiconductor systems in the literature which exhibit a strong non-Arrhenius temperature dependence of ρ at elevated temperatures. Very often, it is claimed in these cases that the underlying transport mechanism is the VRH transport mode.³⁻⁶ However, one should keep in mind that the VRH regime in semiconductors is usually valid only for extremely low temperatures when the thermal energy kT is much smaller than the width σ of the energy distribution of impurity levels (illustrated in Fig. 1), which is not the case in most semiconductor systems at elevated temperatures. Therefore one must consider other transport mechanisms for explaining the corresponding experimental data. The most natural approach is to seek for an explanation in the regime of charge carrier transport via extended band states, where the carriers are supplied by thermal activation from impurity states, as this transport regime is usually valid in doped semiconductors in the relevant temperature range. The possible occurrence of a strong non-Arrhenius temperature dependence of ρ in the case of traditional band charge transport is the main message of this letter.

In general, electrical resistivity in the band transport regime can be represented by

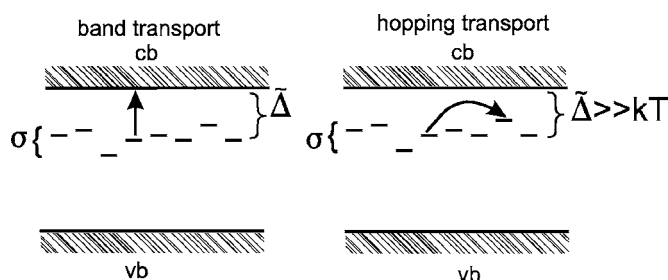


FIG. 1. Left: band transport regime, right: hopping regime where Δ is the activation energy, $\tilde{\Delta}$ is the energy spacing between the localized states and the extended band states, and kT is the thermal energy.

^{a)}Electronic mail: christoph.michel@physik.uni-marburg.de

$$\rho = (ce\mu)^{-1}, \quad (1)$$

where e is the elementary charge, c is the concentration of charge carriers in transport states, and μ is their mobility. For p -type (n -type) semiconductors, the transport states are the extended band states for holes (electrons) in the valence (conduction) band. In such states charge carriers move as free particles with an effective mass.

In semiconductors, the mobility of the carriers via extended states depends comparatively weakly on temperature (i.e., weak power-law form) due to the temperature dependence of scattering cross sections, e.g., in scattering by impurities ($\mu \propto T^{3/2}$) below about 40 K and in scattering by phonons ($\mu \propto T^{-\gamma}$ with $\gamma > 0$) above about 80 K in GaAs.⁷ The carrier mobility cannot therefore be in any sense responsible for the observed, strong non-Arrhenius behavior of ρ .

Hence the only factor in Eq. (1), which can be responsible for the observed temperature dependence, is the concentration of charge carriers c in the transport-carrying band. The crucial question then is why the temperature dependence of this concentration can be non-Arrhenius if charge carriers are supplied into the extended bands by thermal activation from acceptor (donor) states. Two possible disorder-related explanations in the framework of the band transport regime shall be discussed in the following. In scenario 1, the energy levels of holes (electrons) on acceptors (donors) have a broad energy distribution, and in scenario 2, the density of states (DOS) of the extended band states in the vicinity of the band edge possesses a low-energy exponential tail.

Both a distribution of dopants as well as an exponential tail of the DOS lead to a nonlinear shift of the Fermi level as a function of temperature and thus result in a non-Arrhenius temperature dependence of the resistivity.

We will address in what follows the case of holes in the valence band of a semiconductor with zinc blende or diamond structure. Calculations for electrons can be carried out in the same manner and yield similar results. The carrier concentration is calculated according to

$$c = \int_{-\infty}^{E_V} \tilde{D}(E) F^h(E) dE, \quad (2)$$

where $F^h(E)$ is the Fermi distribution of holes and $\tilde{D}(E)$ is the DOS of the valence band. Defining $D(E)$ as the ideal square-root-like DOS in the approximation of parabolic valence bands taking into account both heavy holes and light holes, disorder of the band states can be included by adding an exponential tail yielding

$$\tilde{D}(E) = \begin{cases} D(E), & D(E) \geq \alpha \\ \alpha \exp\left(-\frac{(E - D^{-1}(\alpha)) \ln 2}{\delta}\right), & D(E) < \alpha, \end{cases} \quad (3)$$

where α is the onset of the tail, D^{-1} is the inverse function of the ideal DOS, and δ is a damping in form of a half-width energy, which is treated as a free parameter. In the calculation corresponding to the first scenario an ideal square-root-like DOS was used, i.e., $\alpha = 0$. In the second scenario, α was nonzero and δ was varied.

The concentration of charge carriers c is decisively determined by the position of the Fermi level. The latter is calculated using the neutrality condition. In the second case of a deltalike DOI of the acceptor, the Fermi level is given by the neutrality condition in the form

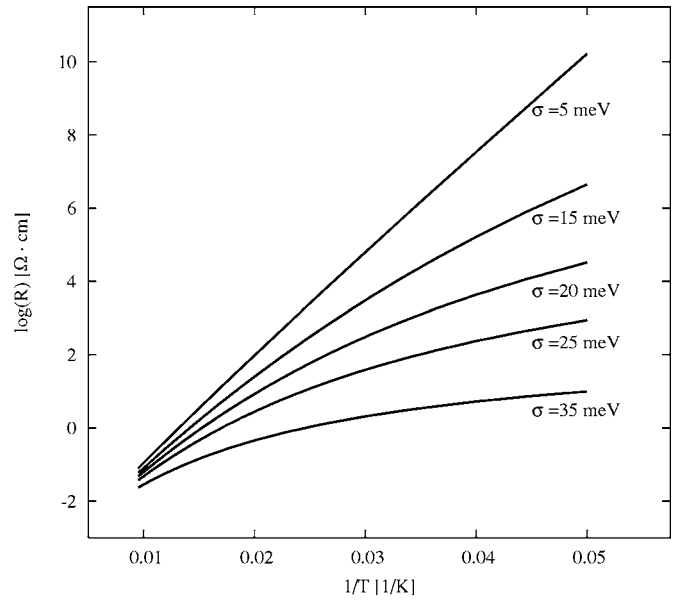


FIG. 2. Logarithmic plot of the calculated resistivity vs $1/T$ for a $\text{Ga}_{0.998}\text{Mn}_{0.002}\text{As}$ sample for different values of σ as indicated in the figure. The valence band DOS has the ideal square-root shape.

$$\int_{-\infty}^{E_V} \tilde{D}(E) F^h(E) dE = N_A F^e(E_A), \quad (4)$$

where N_A and E_A are the concentration and the energy depth of acceptors, respectively, and $F^{h(e)}(E)$ is the Fermi distribution of holes (electrons). With the assumption of a broad DOI of the acceptor states (first scenario), the right-hand side of Eq. (4) has to be replaced by

$$c = \int D_A(E) F^e(E) dE, \quad (5)$$

where $D_A(E)$ is the DOI of acceptor states. We assume this distribution to be Gaussian

$$D_A(E) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(E - E_A)^2}{2\sigma^2}\right) \quad (6)$$

centered at $E_A = 110$ meV above the unperturbed valence band edge. The width σ of this distribution is treated as a free parameter.

Results of calculations for the first scenario using Eqs. (1)–(6) are shown in Fig. 2 for different values of σ . For the narrowest band the temperature dependence of the resistivity can be approximated by the Arrhenius law. With increasing broadening of the acceptor DOI the results of calculations for the temperature dependence of the resistivity deviate more and more from the Arrhenius behavior. The broadening of the acceptor distribution leads to a nonlinear temperature dependence of the Fermi level. The broader the energy distribution of holes on acceptors, the weaker is the temperature dependence of the concentration of thermally activated holes in transport states at the valence band edge. Therefore, the introduction of disorder into the reservoir of charge carriers, i.e., on the right-hand side of Eq. (4) (energetically distributed acceptor levels), can cause the non-Arrhenius temperature dependence of the resistivity although no disorder is present in the transport-carrying band.

The theoretical curves for the resistivity are very sensitive to the choice of the parameter σ , as can be seen from

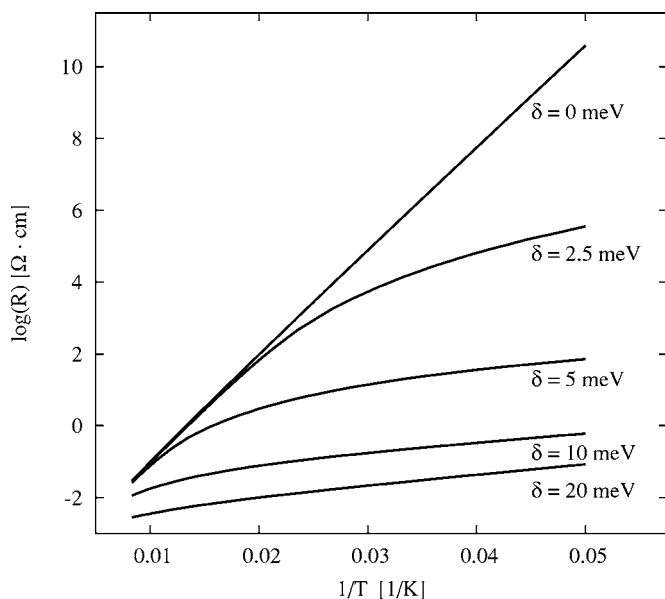


FIG. 3. Logarithmic plot of the calculated resistivity vs $1/T$ for a $\text{Ga}_{0.998}\text{Mn}_{0.002}\text{As}$ sample for different values of δ as indicated in the figure. The energy distribution of the acceptor states is a delta function.

Fig. 2. Changing σ to 20 or to 30 meV leads to an order of magnitude change of the resistivity and a different curvature of the plot. Therefore, for a known impurity depth E_A , the comparison of theory and experiment might allow one to determine the energy width σ of the DOI.

Results of the second scenario obtained using different values of δ in the calculation [see Eq. (3)] are shown in Fig. 3. It can be seen that in the absence of an exponential tail the resistivity shows the usual Arrhenius dependence. With increasing δ the low temperature resistivity drastically drops leading to a non-Arrhenius temperature dependence. The rea-

son for this is similar to that in the first scenario discussed above: The disorder accounted for by the variable extension of the exponential tail enters the neutrality equation Eq. (4) as a modification of the DOS leading to a nonlinear dependence of the Fermi energy with increasing temperature. Again the calculation shows a strong dependence of the shape of the curves on the free parameter δ which allows one (if a broad impurity distribution can be excluded) to determine the extension of such a tail by comparison with experimental data.

Herewith it has been shown that a strong non-Arrhenius temperature dependence of the electrical resistivity can occur in the framework of a traditional band transport mechanism. Therefore, a non-Arrhenius dependence of the resistivity of a semiconductor system alone is no proof of variable-range hopping being the dominant transport mechanism. It is worth noting that this statement is basically independent of the semiconductor material.

The authors are grateful to W. Stolz for valuable comments and discussions. Financial support of the DFG via Project No. KL 1289/4-1 and via the European Graduate College “Electron-electron interactions in solids” is gratefully acknowledged.

¹J. S. Blakemore, *Semiconductor Statistics* (Dover, Mineola, 1987).

²B. I. Shklovskii and A. L. Efros, *Electronic Properties of Doped Semiconductors* (Springer, Heidelberg, 1984).

³S. Bhattacharyya, *Phys. Rev. B* **70**, 125412 (2004).

⁴A. Narsale, Y. P. Ali, U. Bhambhani, V. P. Salvi, B. M. Arora, D. Kanjilal, and G. K. Mehta, *J. Appl. Phys.* **82**, 4228 (1997).

⁵A. Dussan and R. H. Buitrago, *J. Appl. Phys.* **97**, 043711 (2005).

⁶J. Betko, M. Morovic, J. Novak, A. Förster, and P. Kordos, *J. Appl. Phys.* **86**, 6234 (1999).

⁷G. E. Stillman, C. M. Wolfe, and J. O. Dimmock, *J. Phys. Chem. Solids* **31**, 1199 (1970).