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Novel approach for calculating the charge carrier mobility and Hall factor for semiconductor materials

G.V. Colibaba [a,b,*]

[a] Moldova State University, A. Mateevici 60, MD-2009, Chisinau, Republic of Moldova
[b] Kazan Federal University, Kremlevskaya 18, 420008, Kazan, Russian Federation

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ABSTRACT

The additive Matthiessen's rule is the simplest and most widely used rule for the rapid experimental characterization and modeling of the charge carrier mobility. However, the error when using this rule can be higher than 40% and the contribution of the assumed additional scattering channels due to the difference between the experimental data and results calculated based on this rule can be misestimated by several times. In this study, a universal semi-additive equation is proposed for the total mobility and Hall factor, which is applicable to any quantity of scattering mechanisms, where it considers the energy dependence of the relaxation time and the error is 10–20 times lower compared with Matthiessen's rule. Calculations with accuracy of 99% are demonstrated for materials with polar-optical phonon, acoustic phonon via the piezoelectric potential, ionized, and neutral impurity scattering. The proposed method is extended to the deformation potential, dislocation, localized defect, alloy potential, and dipole scattering, for nondegenerate and partially degenerate materials.

1. Introduction

The high accuracy calculation of the charge carrier mobility is an important factor when analyzing scattering mechanisms in various materials. One of the most accurate calculation methods is based on the sophisticated integration of the relaxation time [1]. However, the simpler additive Matthiessen's rule has still been used in many studies for the experimental characterization of mobility and its modeling in various devices [2], despite the fact that the error when using this rule can be as high as 42%. If the difference between the experimental data and the results calculated based on this rule is attributed to an additional unknown scattering effect, then the assumed scattering channel can be misestimated by several times. More exact equations have been proposed [3–5] but these sophisticated equations usually contain additional effective parameters, which are dependent on the properties of materials. Some methods [3,4] only consider the two main scattering mechanisms but several scattering channels must be treated simultaneously in some materials, such as ZnO [6]. A universal high accuracy equation that is suitable for any semiconductor material and any quantity of scattering channels is not available for determining the charge carrier mobility or the Hall factor.

2. Preliminary notes

The widely used parabolic band approximation, isotropic scattering approximation, elastic scattering approximation, and the mutual independence of scattering mechanisms are assumed in this investigation [1]. In the proposed approach, the total mobility (μ_τ) and Hall factor (r_τ) can be calculated as follows [1,6]:

$$\mu_\tau = \frac{q}{m}\langle\tau\rangle, \tag{1}$$

$$r_\tau = \frac{\langle\tau^2\rangle}{\langle\tau\rangle^2}, \tag{2}$$

where q, m, and $\langle\tau\rangle$ are the electron charge, effective polaron mass, and average total relaxation time of the charge carriers, respectively. The Hall factor corrects the mobility and charge carrier concentration (n) using well known equations [1]: $\mu_\tau = R_H\sigma/r_\tau$, and $n = r_\tau/qR_H$ (R_H and σ are the Hall coefficient and conductance, respectively).

Several scattering mechanisms play major roles in carrier transport in bulk and layered materials: polar-optical phonon (po), acoustic phonon via the piezoelectric potential (pe) and via the deformation potential (dp), ionized (ii) and neutral impurity (ni) scattering [1,6]. The formulae

* Moldova State University, A. Mateevici 60, MD-2009, Chisinau, Republic of Moldova.
E-mail address: GKolibaba@yandex.ru.

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