Structurally Complex Two-Hole and Two-Electron Slow Traps with Bikinetic Properties in p-ZnTe and n-ZnS Crystals

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Abstract—Thermal-activation and photoactivation methods were used to ascertain the existence of two-hole traps in p-ZnTe crystals and two-electron traps in n-ZnS. It was found that these traps have a large number of energy states that are grouped in two series of levels: $E_v + (0.46–0.66)$ eV and $E_v + (0.06–0.26)$ eV in p-ZnTe and $E_C – (0.6–0.65)$ eV and $E_C – (0.14–0.18)$ eV in n-ZnS. Both the hole and the electron traps belong to the class of slow traps with bikinetic properties. These traps feature normal kinetic properties in the state with a single trapped charge carrier and feature anomalous kinetic properties in the state with two charge carriers. Multiple-parameter models allowing for a relation of traps in p-ZnTe and n-ZnS to the vacancy–impurity pairs distributed according to their interatomic distances and localized in the region of microinhomogeneities with collective electric fields that repel the majority charge carriers are suggested. The main special features of behavior of electron and hole traps are explained consistently using the above models. © 2004 MAIK “Nauka/Interperiodica”.

1. INTRODUCTION

Methods of thermally stimulated currents (TSCs) and induced extrinsic photoconductivity (IEP) were used to study two-hole and two-electron traps with closely coinciding photoelectric parameters in p-ZnTe and n-ZnS. The thermodynamic properties of intrinsic defects in II–VI compounds suggest that these traps can be formed [1]. The main properties of electron and hole traps are explained assuming that these traps are related to vacancy–impurity pairs, which incorporate the cationic ($V_C$) and anionic ($V_A$) vacancies for the electron and hole traps, respectively. The suggested model concepts of hole and electron traps, when taken as a whole, also include the idea that microinhomogeneities of point defects and macroinhomogeneities in p-ZnTe and p-ZnS crystals affect the characteristic parameters of the traps. It is shown that both the electron and hole centers belong to the class of slow traps. In the state with a single charge carrier, the traps under consideration exhibit normal kinetic properties, whereas these properties are anomalous if two charge carriers reside in the trap.

2. THERMALLY STIMULATED CURRENTS

2.1. Estimation and Control of Characteristic Parameters of the Traps Using Thermally Stimulated Currents

The value of TSC caused by thermal ionization of a slow trap (the ratio between the rate of capture of a majority charge carrier by a trap and the recombination rate $R \ll 1$) is given by [2]

$$I(T) = I_0 \exp\left(-\frac{E_i}{kT}\right) \times \exp\left[-\frac{\gamma N_{eff}S_i(kT^2)}{\beta E_i} \exp\left(-\frac{E_i}{kT}\right)\right].$$

(1)

where

$$I_0 = \gamma \hat{\theta} N_{eff} S_i n_{i0},$$

(2)

$E_i$ is the ionization energy for the trap; $S_i$ is the capture cross section for a majority charge carrier; $n_{i0}$ is the initial number of charge carriers in the trap; $\hat{\theta}$ is the thermal velocity of charge carriers; $N_{eff}$ is the effective density of states in the band of majority charge carriers; $\beta$ is the rate of heating the sample when the TSC spectrum is recorded; and $\gamma$ is a factor that depends on the geometric parameters of the sample, the external electric field, and on the charge, lifetime, and mobility of majority charge carriers.

In the initial stage of thermal ionization of the trap, the contribution of the second exponential function in expression (1) to the dependence $I(T)$ is small. The increase in TSC is exponential at this stage. This result was used to introduce into practice the methods for determining the energy $E_i$ from the slope of the straight line [3, 4],

$$\log I(T) = \log I_0 - \frac{E_i}{kT},$$

(3)
and the cross section from the formula [5, 6]

\[
S_t = \frac{\beta I_{ext}}{\theta N_{el} \Delta T}.
\]  

(4)

Formula (4) follows from expressions (2) and (3) when the quantity \( I \) is replaced by its extrapolated value \( I_{ext} \) at the point of intersection of straight line (3) with the vertical axis \( T^{-1} = 0 \), the concentration \( n_0 \) is replaced by the ratio \( \theta / \beta \), and the area \( \theta \) under a specific TSC band is replaced by the band half-width \( \Delta T \). The equality \( \theta = \Delta T \) is valid for a model (pure triangular) TSC band with the amplitude \( I_{max} = 1 \) (in arbitrary units) and the pedestal width \( \Delta T_0 = 2 \Delta T \). Replacement of the area \( \theta \) by \( \Delta T \) when estimating \( S_t \) from formula (4) introduces an error no larger than 10%; this error only affects the factor multiplying the quantity that defines the order of magnitude of the cross section \( S_t \). In the case of complex TSC spectra, the half-width \( \Delta T \) can be estimated as double the width of the low-temperature portion of an elementary band separated using the "thermal decontamination" method [7].

Direct estimation of \( I_{ext} \) includes procedures for normalizing the TSC spectrum and extrapolating the straight line \( \log I = f(T^{-1}) \) to the vertical axis \( T^{-1} = 0 \). A simple expression for the estimate of \( I_{ext} \) follows from the shape of the right-angled triangle (Fig. 1, inset) in the coordinate system \( [\log I, 10^{-1}/T] \). The base of the triangle lies in the horizontal axis \( \log I = 0 \) and passes through the peak of the TSC band. The length of this base is \( 10^{1}/T_0 \) and equals the abscissa of the point of intersection of the horizontal axis with the straight line defined by expression (3); the extrapolated portion of this straight line forms the hypotenuse of the triangle. The length of the vertical cathetus is equal to \( \log I_{ext} = 10^{1}/T_0 \tan \alpha \) (Fig. 1, inset). The tangent of the angle of inclination of straight line (3) to the horizontal axis defines \( E_t \). Another result following from the expression for \( \log I_{ext} \) is of practical importance (and was hitherto unknown): \( \tan \alpha \) (via the quantity \( I_{ext} \)) makes it possible to determine the cross section \( S_t \) of capture of charge carriers by slow traps [see formula (4)].

Transition from the TSC spectrum given by (1) to the point of its maximum, where \( T = T_m = \frac{d I}{d T} = 0 \), yields the approximate equality [8]

\[
\log \frac{S_t}{S_0} \equiv \frac{E_t}{kT_m} \log e.
\]  

(5)

In dimensionless coordinates \( [\log \frac{S_t}{S_0}, \frac{E_t}{kT_m}] \), this equality represents a universal diagram for characteristic parameters of both slow traps (\( E_t, S_t \)) and corresponding thermally stimulated bands (\( \beta, T_m \)) in semiconductors and insulators. The parameter \( S_0 \) is defined as \( S_0 = \beta / \theta N_{el} T_m \).

The accuracy of estimates for parameters \( E_t \) and \( S_t \) can be judged by checking whether these estimates are consistent with diagram (5) and whether the shape of the experimental bands coincides sufficiently with that of the bands given by (1) and calculated using the above parameters.

2.2. TSCs and Characteristic Parameters of the Traps

Integrated TSC spectra in the temperature range 90–300 K both in \( p \)-ZnTe (Fig. 1, curve \( a \)) and in \( n \)-ZnS (Fig. 2, curve \( a \)) consist of two broad bands. Resolution of these bands into elementary bands (Fig. 1, curves \( b–k \); Fig. 2, curves \( b–d \)) employing the “thermal decontami-