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Empirical Correlations between the Arrhenius' Parameters of Impurities' Diffusion Coefficients in CdTe Crystals

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Abstract. Understanding of self- and dopant-diffusion in semiconductor devices is essential to our being able to assure the formation of well-defined doped regions. In this paper, we compare obtained in the literature up to date the Arrhenius' parameters ($D=D_0\exp(-\Delta E_a/kT)$) of point-defect diffusion coefficients and the I-VII groups impurities in CdTe crystals and films. We found that in the diffusion process there was a linear dependence between the pre-exponential factor, D_0, and the activation energy, ΔE_a, of different species: This was evident in the self-diffusivity and isovalent impurity Hg diffusivity as well as for the dominant IIIA and IVA groups impurities and Chlorine, except for the fast diffusing elements (e.g., Cu and Ag), chalcogens O, S, and Se, halogens I and Br as well as the transit impurities Mn, Co, Fe. Reasons of the lack of correspondence of the data to compensative dependence are discussed.

Keywords: CdTe, impurities diffusion, Arrhenius' equation, compensation effect, Meyer-Neldel rule

1. Introduction

During the last few decades, CdTe crystals have garnered growing interest as multi-functional materials for many applications in the fields of environment, national security, and medical imaging. They also have attracted attention as room-temperature X-ray- and gamma-ray-detectors, and as a substrate for the epitaxial growth of CdHgTe, which is employed in infrared focal-plane-array detectors, among other uses. The physical properties of CdTe usually are modified by foreign atoms introduced during the crystals' growth, or by a post-growth diffusion process [1]. Thus, knowing the parameters of the diffusion of impurities is of great importance in developing these electronic devices.

Four extensive reviews have been published on the diffusion of different impurities in CdTe crystals [1-4]; in many cases, they reveal major discrepancies in the descriptions of the behavior of the same doping agent.

An attempt to find a method of the experimental results reliability estimation was undertaken in [4] where general characteristics of the diffusion process, contained in the Arrhenius' equation

$$D = D_o \exp(-\Delta E_a / kT) \qquad (1)$$

are compared. Figure 1 shows the correspondence between logarithm of the pre-exponential factor D_o and activation energy ΔE_a of various impurities in solid CdTe that was obtained in [4]. The data demonstrate a tendency to linearity but with poor correlation coefficient R^2 value in some cases, probably, due to lack of appropriate experimental data.

Really, it is known that in several diffusion processes for the elemental semiconductors Si and Ge, as well as for the compounds CdS, GaAs, and CdHgTe, among others, it was found that D_o depends exponentially on the ΔE [1, 4-8]:

$$D_o = \exp(-\Delta E_a / kT_o) \qquad (2)$$

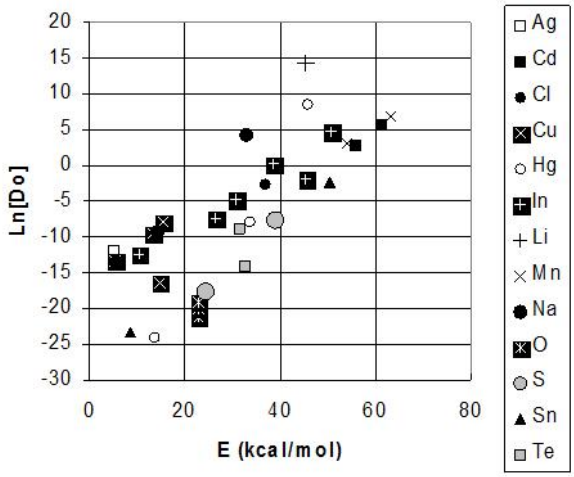

Figure 1 The best linear fits to the yield of solute-diffusion data collected in [4]: Cu: $\ln[D_o] = 0.21E - 14.3$ ($R^2 = 0.06$); Hg: $\ln[Do] = E - 38.8$ ($R^2 = 0.98$); In: $\ln[Do] = 0.40E - 16.9$ ($R^2 = 0.91$); Na: $\ln[Do] = 0.67E - 18.1$ ($R^2 = 0.99$).

This phenomenon has many different names [9] but mostly is referred to as the compensation effect (CEF) and the isokinetic (or isoequilibrium) effect (often called as Meyer-Neldel rule MNR) [1, 4-13], wherein the so-called isokinetic temperature, T_o, is consider as constant for a material, and kT_o is a characteristic energy. Isokinetic temperature, T_o represents a temperature at which all reactions of the series of related processes should proceed at the same rate in a limited temperature range.

The MNR, as well as the compensation rule, often is represented by linear equation 3:

$$lnD_o = a\,\Delta E_a + C \qquad (3)$$

The MNR, an empirical relation, has been found in an extremely wide range of fields [9] and systems, including many different single-crystalline- and polycrystalline semiconductors, in amorphous and organic ones, in ionic-conducting crystals and glasses and others.

The origin of the MNR or CEF is not clear in spite of many attempts to clarify it [9, 12, and 13]. There are several explanations for the MNR in inorganic semiconductors; the phenomenological approach is based on the exponential distribution of the energy barriers [10]. Another one supposes that the freezing-in of donor acceptor-type defects can lead to the applicability of this rule to both band conductors and small polaron-hopping conductors. Next, it was shown that a Gaussian distribution of defect-energy levels or a Gaussian distribution of hopping energies, under specific conditions of the defect's interactions, also leads to this rule [11].

The MNR is only one manifestation of the very general peculiarities of the compensation effect. Various theories have been proposed to explain the CEF in diffusion. According to [5], the linear dependence of $\ln D_o$ on ΔE_a reflects the fact that, under conditions of isobaric heating, part of the heat is consumed by the expansion of the lattice; the other part is used to enhance the diffusion motion. Some theories are based on the enthalpy-entropy interrelationship (enthalpy and entropy compensate for each other because of their opposite algebraic signs in the Gibbs' equation), others on the relation between the entropy of transitions and changes in the energy levels of the transition state, whilst others are founded on the kinetic many-body theory of thermally activated rate-processes in solids [6], due to the existing interrelated kinetic behaviors within a group-rate process. and others [7-11]. Recently Starikov et al had concluded in the vast reviews [12, 13] that in any cases of correlated designed reliable experimental data the MNR-type dependence reveals a valid entropy-enthalpy compensation.

It is interesting to compare the data published up to date on the diffusion of impurities and intrinsic defects in CdTe crystals and films, and to evaluate it according to its correspondence with the findings from MNR or CEF.

2. Self-diffusion in CdTe

One specific feature of admixture diffusion in a binary compound A^2B^6 type is its possible dependence on the volatile component pressure that regulates the content of that material's

vacancies. So, first of all, we consider the possibility of CEF for the components' self-diffusion in the CdTe lattice.

Table 1 presents the Arrhenius parameters of the self-diffusion and chemical diffusion, found in reviews [1-4] and other papers [14-21]. Figure 2 is a graphical presentation of the data,

Table 1. Pre-exponential factor and activation energy of self-diffusion in CdTe

Dopant or defect	$D_{o,\ cm}{}^2s^{-1}$	ΔE_a, eV	Experimental conditions and *analytical method*; type of diffusion profile	Ref.
$\mathbf{Cd_i^{\bullet\bullet}}$	29.4	1.23±0.02		14
$\mathbf{V_{Te}^{\bullet\bullet}}$	**30**	**1.91±0.04**		14
$\mathbf{V'_{Cd}}$	380	1.65		14
$\mathbf{V''_{Cd}}$	2.24×10^4	2.09±0.07		14
$\mathbf{Te_i}$	0.66	0.77±0.07		14
$\mathbf{^{115m}Cd}$	1.26	2.07	973 – 1273 K, P_{Cd} Multi-component self-diffusion profiles	15
$\mathbf{^{109}Cd}$	326	2.67	Above 923 to 1273 K, P_{Cd} (below 923 K the Arrhenius plot cannot describe the experimental results)	16
$\mathbf{^{109}Cd}$	15.8	2.44	Previously Te-saturated compound	16
$\mathbf{^{109}Cd}$ **in CdTe+Al**	1.37×10^{-7}	0.67	1073 - 1173 K, P_{Cd}	16
$\mathbf{^{123}Te}$	1.66×10^{-4}	1.38	773 - 1123 K; Te saturation	16
$\mathbf{^{123}Te}$	$\mathbf{8.54\times10^{-7}}$	**1.42**	923 - 1173 K, previously Cd-saturated compound	16
Cd	4	1,15	823 - 1073 K. *Electrical measurements* Profiles with exponential "tails"	17
$\mathbf{^{109}Cd}$ $\mathbf{(V'_{Cd}\ Cd_i)^x}$	6.67×10^{-2}	2.01	973, 1073-, and 1173 K	18
$\mathbf{Cd_i^{\bullet\bullet}}$	21.7	1.21	" "	18
$\mathbf{V_{Te}^{\bullet\bullet}}$	$\mathbf{5.7\times10^{-2}}$	**1.42**	" "	18
$\mathbf{V'_{Cd}}$	390	1.63	" "	18
$\mathbf{V''_{Cd}}$	2.74×10^3	1.85	Estimated according to the data [16]	18
$\mathbf{Te_i}$	2.04×10^{-2}	0.42		18
$\mathbf{V'_{Cd}}$	5.5×10^{-3}	0.68	CdTe + 5×10^{17} at/cm^3 Al	11
$\mathbf{V''_{Cd}}$	0.011	0.68	CdTe+ 10^{17} at/cm^3 Al	11
$\mathbf{Cd_i^{\bullet\bullet}}$	**0.23**	**0.99**	773 -1173 K *Electrical measurements*	19
Cd	5	1.12	773 -973 K *Electrical measurements*	20
Cd in **CdTe+Cl**	1.5×10^7	2.55	873 –973 K, near Cd saturation	21

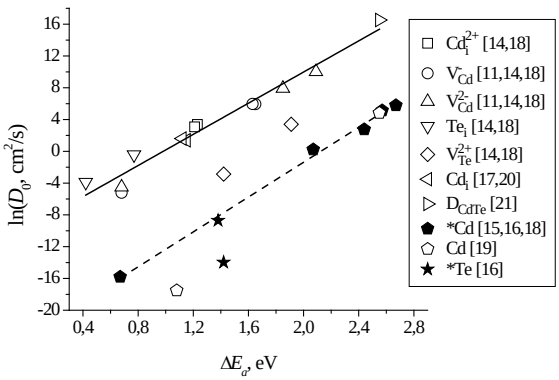

Figure 2 The plot of the pre-exponential constant D_o as a function of the activation energy ΔE_a of self-diffusivity in CdTe crystals. Radiometry data for D_{Cd} and $D_{Te,}$, black points, dashed line: $\ln D_0 = (9.8\pm0.6)\ E_a - (9.6\pm0.8)$, $R^2=0.96$; the charged-point defects calculated diffusivity data, empty points, solid line: $\ln D_0 = (11.0\pm0.3)\ E_a - (23.3\pm0.7)$, $R^2=0.99$.

demonstrating their large dispersion on the whole. However assuming that the results obtained by radiometry in [15, 16, 18], which considered as the most sensitive tool for studying diffusion phenomena in solids, is correct, then we can see the rectilinear correlation for Cd self-diffusivity

data (black points, dashed line). In such case, the Meyer-Neldel rule seems to be adhered to very closely by a good number of independent data-points.

Besides, the calculated by Kröger [14] and specified in [18] data denoted that the self-diffusivity of the charged-point defects, except for $V_{Te}^{\bullet\bullet}$, can be considered as the NMR or CEF linear-dependence (empty points, solid line). The points, excluded from both lines, are distinguished as bold in Table 1. Obviously, the vacancies migrate faster than the total flux of Cd or Te atoms with close slope of the CEF correlations.

For self-diffusion, it is considered that the Gibbs' free energy for the activation of this process, which defines the fraction of delocalized atoms, decreases slightly as the temperature rises. This reflects the fact that the higher the temperature the lower the quantity of energy that is required to delocalize an atom in the lattice due to increasing fluctuations. Consequently, the enthalpy of self-diffusion activation increases slightly with temperature.

3. Diffusion of foreign impurities in CdTe

Table 2 shows the data obtained in literature up to date and in our own studies on the diffusivity of I–VII group impurities in CdTe crystals and films. We took into account also results of the electrical properties measurements as well as via several different approaches to determine their concentrations.

Table 2. Arrhenius' parameters of I-VII group impurities diffusivity in CdTe

Impurity	$D_{o,\ cm}{}^2s^{-1}$	ΔE_a	Experimental conditions; *method of impurity determination*, type of diffusion profile	Reference
Li in **CdTe+Cl**	1.62×10^{6} 4.6×10^{3} 6.0×10^{6}	1.98 1.6 0.33	570 - 700 K Li diffusion from vapor Li diffusion from thin surface layer *Hall constant during layer removal of CdTe, doped by Cl* *p-n transition method* Two diffusion components	22
Na in **CdTe+Cl**	1.18×10^{-6} 8.97×10^{-5} 3.7×10^{-2}	0.25 0.62 1.42	470 – 700 K $[h^{\bullet}] = 10^{9} - 10^{10}$ $[h^{\bullet}] = 10^{11} - 10^{12}$ 700 - 970 K *measuring the Hall constant*	23
***Cu**	3.7×10^{-4}	0.67	370 – 573 K Diffusion from Cu_2Te films two components of diffusion	24
Cu	8.2×10^{-8}	0.64	563-623 K *decrease in thickness of vapor-deposited layers*	25
^{64}Cu	9.57×10^{-4}	0.7	523 - 753 K	26
***Cu**	6.65×10^{-5}	0.57	473 - 673 K	27
Cu	1.7×10^{-6}	0.24	*capacitance transient measurements*	28, 29
Ag	6.5×10^{-6}	0.22	*capacitance transient measurements*	28
***Ag**	3.7×10^{-3}	0.65		30
Ag	164	0.64	*Microscopic observation of CdTe-Ag's boundary movement*	31
***Au**	67	2	873 - 1273 K; *autoradiography*	32
Au in CdTe films	9×10^{-3}	1.7	473 - 723 K, P_{Te2} *Charged-particle, Rutherford back-scattering, and ion-microprobe techniques*	33
Au in CdTe films	4.4×10^{-7}	0,54	673-823 K *Energy dispersive X-ray fluorescence analysis*	34
^{65}Zn	1.39×10^{-9}	0.08	770-1170 K Time-dependent profiles	35
^{65}Zn	4.14×10^{-4} 5.90×10^{-8}	1.21 0.77	823-1223 K, two components of diffusion Fast diffusion Slow diffusion	59
Zn in CdTe films	2.5×10^{-3}	1.30	703 - 793 K *current–voltage characteristics, thin films*	36

***Hg**	3.4×10^{-11} 3.5×10^{-4} 1.0×10^{-11} 3.4×10^{-7}	0.6 1.46 0.36 0.97	433- 676 K, saturated Hg vapor pressure. Two-component profiles with D_1 and D_2 according to erfcz: below 548 K above 548 K below 548 K above 548 K	37
^{203}Hg	0.017 2.84×10^{-13} 2.65×10^{-6}	1.572 0.265 0.789	296 - 733K Dslow, T> 614 K Dslow, T< 614 K Dfast	38
Hg	1.2×10^{-3}	2.0	*Heavy-ion (40 MeV O^{5+}) back-scattering methods*	39
Hg	6.6÷14	1.91±0.16	360 -550 ^{o}C *Proton induced X-ray emission*	40
Al in **CdTe+Cl**	67.6 1.7×10^{4}	1.43 1.73	570-700 K Al diffusion from vapor Al diffusion from thin surface layer *Hall constant during layer removal of Cl doped CdTe*	22
***Ga**	1.75×10^{-2}	1.78	973-1173 K, P_{Cd}	41
^{71}Ga, SIMS	3.1×10^{-3} 5.9×10^{-2}	1.52 1.56	737-1084 K Ga*, 623-738 K SIMS. Mechanism A, $\mathbf{V_{Cd}}$ Mechanism B, interstitial or dislocation	42
In	0.041	1.62	Vacuum, 723-1273 K *p-n transition method*	43
***In**	8×10^{-2}	1.62	Vacuum, 723 - 1273 K	44
***In**	9×10^{-3}	1.34	928 - 973 K ; P_{Te2} ,	45
^{114m} In	3.3×10^{-4} 1.71×10^{-3}	1.1 1.5	873-1173 K ; P_{Cd} c.s.**	46
In in **CdTe+Cl**	1.17 1.4×10^{-1} 4.02×10^{-6}	1.68 1.98 0.46	583 - 665 K $[h^{\cdot}] = 10^{16} \div 2 \times 10^{16}/cm^3$, $[h^{\cdot}] = 2\times10^{14} \div 3 \times 1\ 0^{14}/cm^3$, $[h^{\cdot}] = 10^{9} \div 10^{10}/cm^3$. *Hall-effect measurements*	23
^{114m}In	117÷1.64 $(6.48\div2.72)\times10^{-4}$ $(3.22\div1.47)\times10^{-4}$ 1.44÷2.98	2.21±0.04 1.15±0.08 1.13±0.03 1.82±0.09	473-1073 K Above 673 K, $P_{Cd,}$ In surface layer Above 673 K, $P_{Te2,}$ In surface layer 673-1073 K, In/Te alloy 873-1073 K, In/Cd alloy	47
In	4×10^{-2}	0.9	Around 473K *Admixtures Introduced by Ion Bombardment*	48
***Tl**	4.09×10^{-4} 4.07×10^{-4}	1.13 1.33	873-1173K c.s.** $P_{Cd,\ max.}$	49
^{71}Ge	1.64×10^{-3} 1.28×10^{-8}	2.07 1.03	903-1203 K c.s. ** $P_{Cd,\ max.}$	50
^{113}Sn	8.3×10^{-2} 6.9×10^{-11}	2.2 0.38	1020 -1190 K c.s., two-component profiles $P_{Cd,\ max.}$	51
^{32}P	1.8×10^{-3}	1.99±0.10	873 – 1173 K; P_{Cd}, P_{Te2}	52
Bi	1×10^{-10}	0.3-0.4	473- 723 K. *Ion microprobe technique*	33
O	2×10^{-9} 5.6×10^{-9} 6×10^{-10}	0.83 1.27 0.29	n, below 923 K p, below 923 K n, p, above 923 K *Mass-spectrometry* Time dependent diffusivity	53
S	$(2.5\pm1.1)\times10^{-8}$ $(4.9\pm4.6)\times10^{-4}$	1.06±0.04 1.7±0.2	645 - 948 K; a mixture of CdS and CdTe powders. Two mechanisms: Below 763 K Above 763 K *SIMS*	54
***Se**	1.7×10^{-4}	1.35	973-1273 K	55
^{36}Cl	0.071÷2.4 $(1.05\div5.9)\times10^{-2}$	1.60± 0.07 1.43± 0.14	793 - 1073 K $P_{Cd,\ max}$ $P_{Cd,\ min}$	56
^{36}Cl	$(3.3\pm 1.0)\times10^{-2}$	1.32±0.1	473-973 K The profiles comprised 4 parts	57

	$(4.5\pm 1.0)\times10^{-6}$ $(3\pm 1)\times10^{-10}$ $(2.5\pm 1.6)\times10^{-13}$	1.14±0.1 0.89±0.1 0.63±0.1		
***Br**	$(2\pm2)\times10^{-12}$ $(6\pm2)\times10^{-13}$ $(3\pm1)\times10^{-14}$ $(8\pm2)\times10^{-15}$	0.14±0.05 0.2±0.1 0.18±0.05 0.26±0.06	The profiles comprised 4 parts	58
***I**	$(7 \pm 3)\times10^{-11}$ 2.1×10^{-13} $3.8\pm1.2\times10^{-14}$ $2.1\pm1.6\times10^{-15}$	0.21 0.29 0.28 0.28	The profiles comprised 4 parts	59
I	10^{-8}	0.4	293 - 473 K *Changes in the electrical conductivity of I-bombarded samples* Diffusion via grain boundaries	48
^{54}Mn	22.5 ÷ 3.3 $(1.12\div 9.12)\times10^{3}$ 6.5÷6.26	2.33±0.09 2.76±0.18 2.33±0.14	773 - 1073 K, P_{Te2} 873 - 1073 K, P_{Cd} 773 – 1073 K	60
Mn	 $6{,}41\times10^{-4}$ 1,55 $8{,}74\times10^{-7}$	 1,55 2,13 1,35	673 – 873 K Cd/Te = 2.5 Cd/Te = 0.5 Cd/Te = 1.7	61
***Fe**	1.16×10^{-5}	0.77	900 -1173 K	62
***Co**	3.8×10^{-8}	0.75		63

*- radiotracer experiments c.s.** - congruent sublimation

These experimental data have been determined through a variety of techniques, in different temperature intervals, and in various doping conditions. According to the literature, the diffusion of impurities in CdTe and CdTe-based crystals occurred in many different forms: by interstitials or vacancies, in neutral or charged forms, by dissociative mechanisms and individually or interacting with intrinsic defects, by dislocations or grain boundaries. Many methods have been explored to introduce controlled amounts of the dopants into the crystals, such as from a deposited on surface metallic or metallic telluride layer, from a vapor phase in vacuum or at the pressure of the components, and from an ion-implanted source. In publications on the diffusion in CdTe, many different terms are used to describe the impurities' behavior under different experimental conditions: they include the tracer diffusion of atoms and ions, the diffusion of defects, chemical diffusion, and ambipolar diffusion. Though, as one can see in Figure 1, part of these data had demonstrated the linearity in whole.

According to the published data, the $\Delta E_{\mathbf{a}}$ values range over a wide interval from near zero to 2.76 eV [60]. The last value considerably exceeds the band-gap of CdTe, ΔE = 1.5 eV, confirming the existence of diffusing atoms in an excited state with the energy for the process that is much larger than that of a typical excitation.

Reviewing the data in Table 2, one should pay attention to evidence pointing towards a change in the slope of the Arrhenius' correlation within a certain temperature range (at 548 [37] and 614 K [38] for Hg diffusion; at 743 [42] and 673 K [47] for Ga and In, correspondingly, at 928 K [53] and at 753 K [54] for O and S, correspondingly). The underlying reason for these observations is not clear, however, it may be connected with structural transformations in the lattice.

3.1. Diffusion of isovalent and IB Group fast impurities

First of all, let us compare the data in Figure 1 with a possible CEF dependence for diffusivity of cation isovalent impurities in CdTe, namely Hg and Zn (Figure 3a).

Diffusion of Hg in CdTe crystals was studied both by radiometry in [37, 38] and two other methods (heavy-ion (40 MeV O^{5+}) back-scattering [39] and proton induced X-ray emission [40]). The two last ones proposed higher (1.9 - 2.0 eV) the activation energy value in comparison with one obtained in [37, 38] by radiotracers. The difference between these two groups of experimental techniques is observation in first case of two-component profiles of Hg diffusivity with D_1 and D_2 according to erfcz. It is why a linear approximation is considered only for the radiometry data with

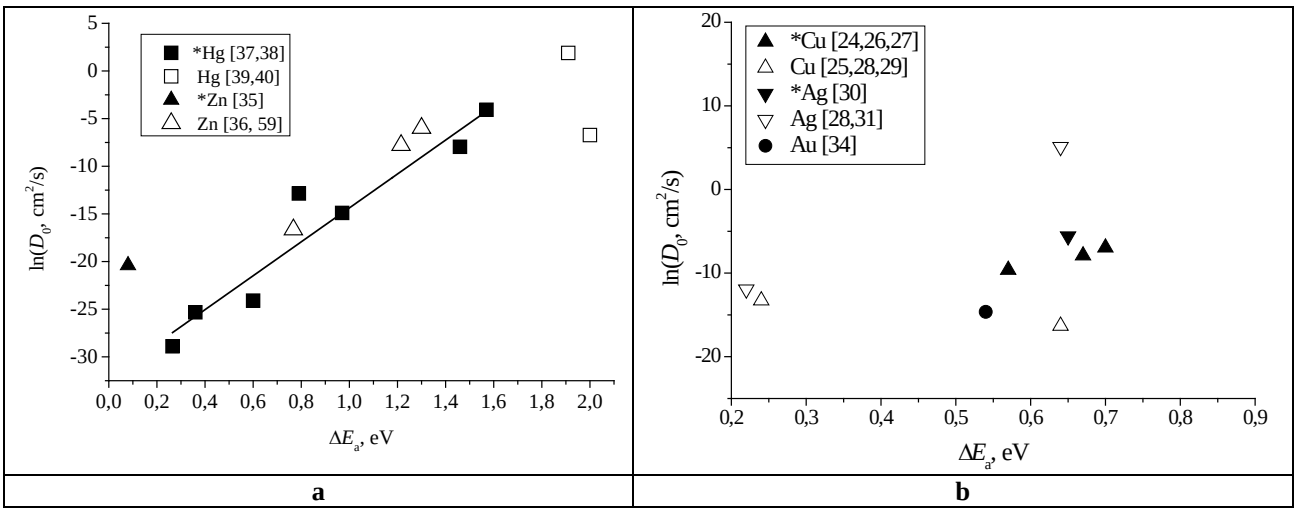

Figure 3 CEF correlation for: a – Hg diffusion in CdTe crystals, $\ln D_0 = (18\pm2)\ \Delta E_a - (32\pm2)$, R^2=0.91; b – IA group impurities Cu, Ag and Au. The various black symbols represent those from the corresponding radiotracer study.

equation $\ln D_0 = (18\pm2)\ \Delta E_a - (32\pm2)$, R^2=0.91, that can be treated as good fit of the experimental data.

Fig. 3a contains also few data for another isovalent impurity Zn, diffusivity of which in CdTe remains discussable [3]. Complication of receipt of reliable Arrhenius' data is caused by a few reasons. It was obtained in [35, 59] a complex multi-diffusion process (time- and mass-dependent Zn diffusivity) that needs to be taken carefully into consideration. Besides, it has been shown in [64] that after diffusion anneals with a pure Zn source in the temperature range 823–973 K, the slice took on a curved shape, which did not occur outside this temperature range. This was due to a differential stress set up across the slice which was relieved by brittle fracture at temperatures below 873K and by ductile slip at temperatures above this value. As result the proposed in [64] experimental data on temperature dependence of Zn diffusivity can't be described by Arrhenius' equation. Therefore the possibility to determine CEF or NMR correlations for Zn in CdTe based on the published data seems unreasonable.

Contrary to Hg and Zn, the noble elements Cu, Ag and Au are rather likely undesirable impurities in CdTe crystals as fast electrical active dopants causing devices electrical instability even near room temperature. For fast diffusing species such as Cu and Ag the activation energy is less than 0.7 eV, implying that interstitial atomic movement is the dominant diffusion mechanism. Results of the diffusion of Cu in CdTe single crystals study in the temperature range 473–673 K using a radiotracer sectioning technique led to conclusion in [27] that complex diffusion occurred via a defect of the form $(Cu_iCd_v)'$. The major portion of the activation energy (0.57 eV) for the diffusion was taken up in the formation of the defect rather than in its migration through the lattice. A much faster diffusion mechanism (≈100 times faster), which did not show any consistent behaviour with temperature, was also observed in the diffusion profiles [27].

For slow diffusing species like Au, E_a reaches 2 eV, and vacancy diffusion is probably the dominant mechanism**.**

As one can see in Figure 3b, there is no any evidence for the CEF- or MNR-approach to the data. It seems that the reason of that is not small statistic or low apparatus sensitivity or other typical experimental difficulties but rather "abnormall" behavior of them in some cases. According to recent publications [65-69] at temperatures ranged 700–900 K the diffusion of Cu, Ag, Au in CdTe exhibits anomalous concentration profiles (uphill) depending upon the external conditions during diffusion; these anomalies essentially reflect the profile of the deviation from stoichiometry. As evident, there is considerable variation in the pre-exponential factor of copper diffusion, while values of the activation energy are much closer. Uphill diffusion in CdTe, i.e., impurities diffuse against their own concentration gradients, was also observed for the impurities Ni, Pd, K, Mn, and Co [68].

Besides, using radioactive Ag, Tregilgas et al. [70] found that Ag segregates to the surface region of CdTe during exposure to ambient light. This phenomenon occurs while the sample is held at room temperature, and is not induced by localized heating or by surface chemical reactions complicating estimation of the diffusion coefficients.

3.2. Diffusion of IA, IIIA and IVA Groups impurities

It is of interest that most of the Arrhenius'data based on electrical measurements in [22, 23] for the diffusivity of Li (except for one point), Na, and Al in doped with Chlorine CdTe crystals can be described by the equation $\ln D_0$= (16.7±0.5) ΔE_a - (19±1) with high reliability R^2=0.99, (Figure 4a, solid line). A linear approximation by $\ln D_0$ = (11±1) ΔE_a - (28±2), R^2=0.97, (Figure 4a, dotted line) demonstrate also diffusivity data of Group-IV impurities Ge and Sn.

According to Table 2 it was paid comparatively most attention to the study of diffusion of IIIA Group impurities, especially In. The radiometry data [44-47] became a base for the equation $\ln D_0$ = (11±1) ΔE_a - (21±2), R^2=0.85 that is in good agreement with Arrhenius' parameters for D_{In} [23, 43, 48] obtained by other techniques (Figure 4a, dashed line). Besides, the data for diffusivity of Ga and Tl also are situated near the approximation for the In diffusivity characteristic data. Mainly, all data about the diffusion of group-III elements lie on this line. Therefore, we can draw conclusion about the existing of linear CEF-type correlation in the wide list of the experimental data of the IIIA group impurities diffusion in the CdTe lattice.

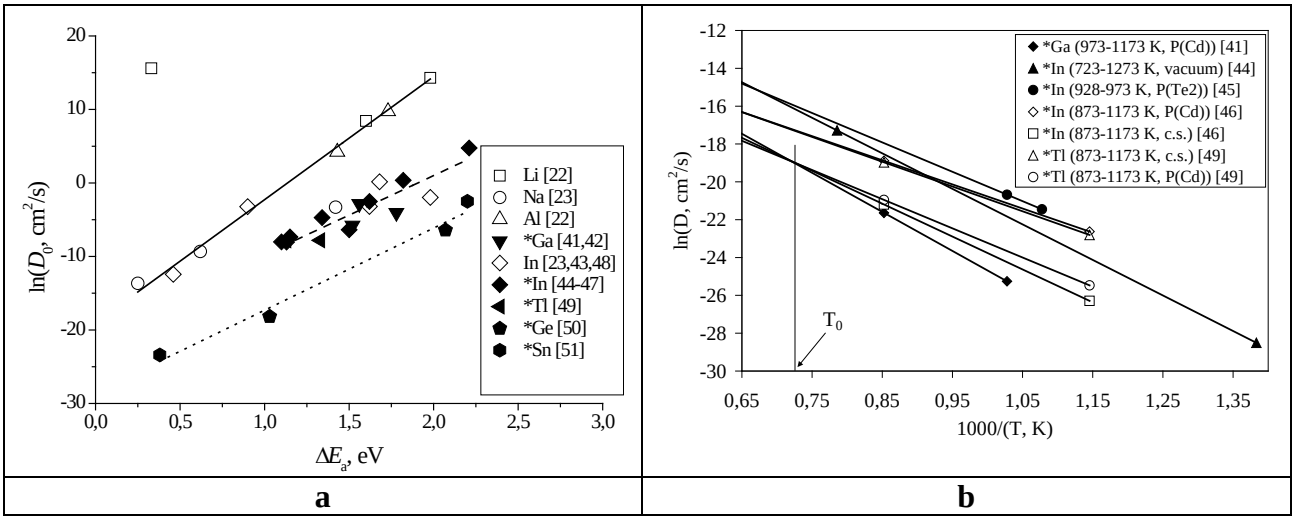

Figure 4 a) The plot of the ln D_o versus ΔE_a for the diffusivity of the Groups I, III and IV impurities in CdTe crystals and thin films. The best fit for determined by the p-n transition method for Li, Na and Al diffusivity (besides the one) according to Hall constant studies [22, 23], solid line: $\ln D_0$ = (16.7±0.5) ΔE_a - (19±1), R^2=0.99. Radiotracer data for IIIA impurities (black points, dashed line): $\ln D_0$ = (11±1) ΔE_a - (21±2), R^2=0.85. Ge and Sn diffusivity radiotracer data (dotted line): $\ln D_0$ = (11±1) ΔE_a - (29±2), R^2=0.97. b) Diffusivity of III Group impurities in CdTe crystals vs reciprocal temperature according to the radiotracer data. The symbols indicate the experimental temperature range.

Attempt to determine the so-called isokinetic temperature T_o using the array of III Group diffusivity radiometry data is illustrated by Figure 4b. Though three temperature dependencies of In, Ga and Tl diffusivity intersect in the same point at T = 1390 K (i.e. in CdTe molten state), it can't be a solid base for a conclusion about the data fit to the NMR because one can obtain another an intersection point at near 1240 K. Obviously, one needs more precise experimental data to determine the isokinetic temperature.

3.3. Diffusion of Halogens and Chalcogens

Comparing various results for the same impurities, one sees that progress in determining the dopant content led to conclusions about the existing of rather complex diffusion profiles. Thus, according to [56-59], the profiles of halogens (Cl, Br, and I) comprise four parts that can be treated as the sum of four complementary error functions. Assuming that a change in the diffusivity mechanism is accompanied with the CEF correlation between pre-factors D_o and ΔE_a, all the Arrhenius' parameters were used for the graphical analysis (Figure 5, a). However, only the data for

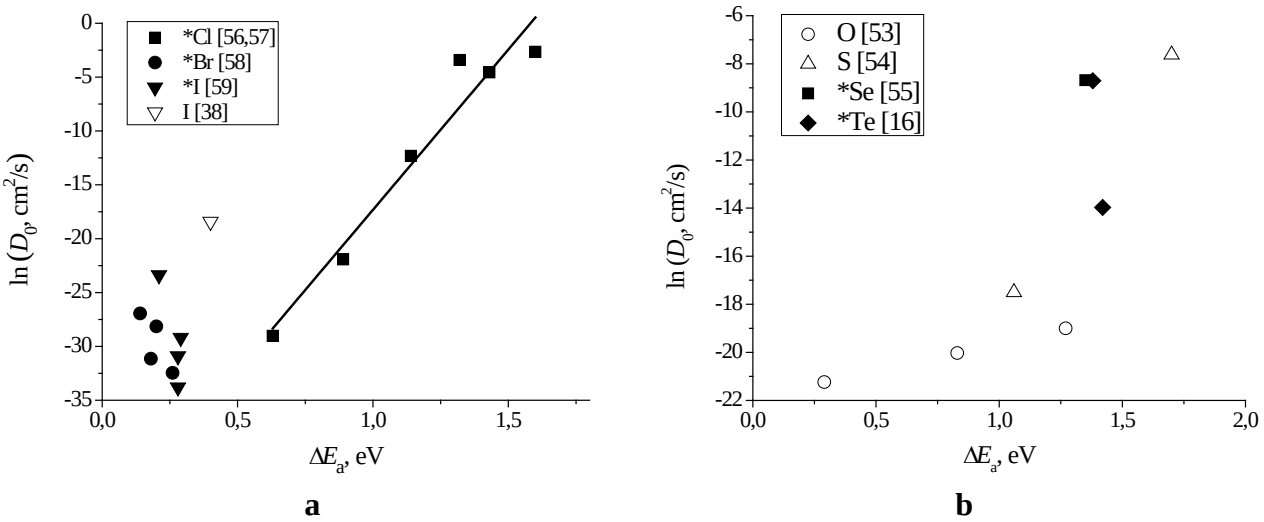

Figure 5 The plot of the pre-exponential factor D_o vs. activation energy ΔE_a of diffusivity of halogens (a) with a linear dependence for the Cl data as $\ln D_0 = (29.8\pm3.5)\ \Delta E_a - (47.3\pm4.3)$, $R^2=0.9$ and chalcogens (b). The black symbols represent those from the corresponding radiotracer experiments.

chlorine diffusivity of [56, 57] corresponded to the CEF and unexpectedly, far from CEF are proposed in [58] data for the bromine and iodine. The reason of that probably was shown in [71] where was obtained that the iodine diffusion caused heterogeneity of the CdTe, so forming a discontinuous phase of randomly distributed particles. Obviously, the concentration of the diffusant in particular regions of the slice complicated the profiles and, correspondently, their interpretation.

The data are highly scattered also for the diffusivity of the chalcogens, O, S, Se, and Te (Figure 5, b). We can suggest some reasons for this. Foremost, there are differences in the analytical methods used. Further, the profiles obtained usually were complex, leading to difficulties in unambiguously calculating the diffusivity. So, as it was noted in [54], a flat- or shallow peak-region in the diffusivity profiles for sulfur can be caused by out-diffusion during cool-down or by quenching from the diffusion-annealing temperature.

3.4. Diffusion of Transit d-Elements

The published data according diffusivity of Mn, Fe and Co at first sight demonstrate satisfactory linearity (Figure 6). However there is no undoubted evidence of their correspondence to NMR or CEF. At the same time similar to most of the previous cases it should be concluded about necessity of modern precise reinvestigation of the impurities behavior (the mechanism of motion and velocity) in defined temperature ranges.

In total, the essential dispersion of most of the diffusivity parameters presented in Table 2 is not surprising. Analyzing the reasons for the scatter of all the published data, we must take into account the thermodynamic- and structural-specificity of the studied specimens. Many cited papers emphasize the surface destruction after certain annealing that is ruled by the duration of annealing and the components' ambient pressure. Besides, it is known that impurities in CdTe can be trapped by tellurium (or cadmium) precipitates as well as by inclusions due to segregation during annealing

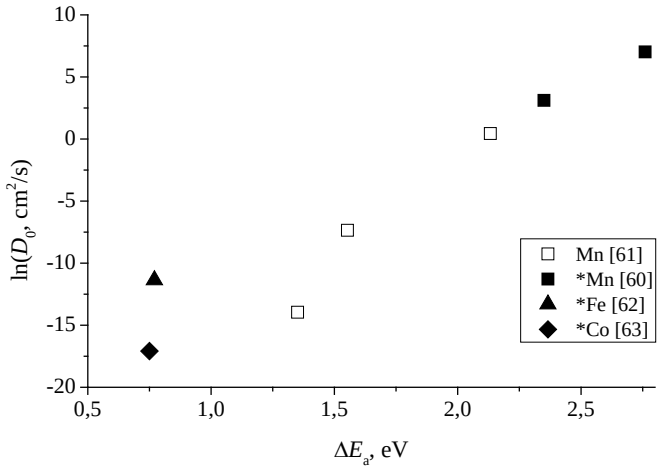

Figure 6 Correlation between ln D_o and ΔE_a for Mn, Fe and Co diffusivity in CdTe.

or quenching [59,72]; that can be one of the reasons for the complicated profiles. In some cases, the experimental results below certain critical temperatures are not described by the Arrhenius' plot which was extrapolated from the high-temperature data (e.g., see [16, 47, and 64]). It is thus difficult to rely upon the best linear approximation.

It must be stressed that successful usage of the CEF or MNR concepts needs first of all reliable experimental data [9, 12, 13]. The ability of them to give meaningful results is linked to the quality of the measurements and approximations errors, but in mind of [9, 12, 13, 73] it appears that no genuine physical effect or fundamental relationships or universal quantities underlie its applicability.

4. Conclusions

We attempted to find linear correlations between the logarithms of the pre-exponential factor ($\ln D_0$) and the activation energy (ΔE_a) of impurities diffusivity in CdTe, known as the compensation effect (CEF) or the Meyer–Neldel rule (MNR). For this work, we used the data array of published up to date the Arrhenius' parameters of self-diffusivity and the diffusion of Group I-VII impurities in the CdTe lattice. A wide scatter of ΔE_a data, and especially D_0, for certain doping elements may reflect possible experimental difficulties caused by the nature of the compound, which consists of volatile components, rather than the incorrectness of the analytical methods were used. In some cases, an apparent scatter may indicate that the diffusant can migrate simultaneously via several different mechanisms depending of external experimental conditions that complicate the erfcz function and the Arrhenius' equation application.

Nevertheless, linear dependences, corresponding to the CEF, were obtained for the diffusion of point defects and for Cd's self-diffusivity (as well as for the isovalent impurity Hg), for the donors from Group III (Ga, In, Tl), for Cl from Group VII and for the amphoteric elements Ge and Sn (Group IV); in all cases, the fits were satisfactory. The correlations can be interpreted as evidence of an inter-relationship between the enthalpy and entropy of the diffusion processes, which is believed to be a major contributor to the compensation effect.

On the contrary, the data for the fast diffusing elements Cu, Ag and Au, donors bromine, iodine and the anion-isovalent impurities chalcogens O, S, and Se did not allow us to reach conclusions about the CEF or MNR in their cases as well as for magnetic impurities Mn, Co and Fe.

The lack of reliable experimental data, unfortunally, prevented us from deducing the isokinetic temperature, $T_{o,}$ at which all rate coefficients are equal. Thus, the correspondence of the parameters of the impurities' diffusivity with the Meyer-Neldel rule remains questionable and needs more attention of researchers. On the other side, the MNR or CEF concept may be a useful interpretation tool when trying to co-ordinate systematical experimental data.

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