

Donor impurity incorporation during layer growth of Zn II-VI semiconductors



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ABSTRACT

The maximum halogen donor concentration in Zn II-VI semiconductors during layer growth is studied using a standard model from statistical mechanics. Here the driving force for incorporation is an increase in entropy upon mixing of the donor impurity into the available anion lattice sites in the host binary. A formation energy opposes this increase and thus equilibrium is attained at some maximum concentration. Considering the halogen donor impurities within the Zn II-VI binary semiconductors ZnO, ZnS, ZnSe and ZnTe, a heat of reaction obtained from reported diatomic bond strengths is shown to be directly proportional to the log of maximum donor concentration. The formation energy can then be estimated and an expression for maximum donor concentration derived. Values for the maximum donor concentration with each of the halogen impurities, within the Zn II-VI compounds, are computed. This model predicts that the halogens will serve as electron donors in these compounds in order of increasing effectiveness as: F, Br, I, Cl. Finally, this result is taken to be equivalent to an alternative model where donor concentration depends upon impurity diffusion and the conduction band energy shift due to a depletion region at the growing crystal's surface. From this, we are able to estimate the diffusion activation energy for each of the impurities mentioned above. Comparisons are made with reported values and relevant conclusions presented.

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1. Introduction

The four zinc chalcogenides ZnO, ZnS, ZnSe and ZnTe, comprise an important group of semiconducting materials. Each in the list either are currently in use or are prospects for future applications within semiconductor based electronic devices. The wide band gap compound ZnO holds promise as a blue/UV LED material [1] and recently, ZnO nanowires of high quality have been produced [2]. ZnS thin films have been successfully *n* doped [3] and with a band gap of around 3.6 eV, this material could have LED applications similar to those of ZnO. ZnS has also been used as a cap for strongly luminescing CdSe nanocrystals [4]. In addition to thin films, isotropic ZnS crystals have been successfully grown [5] and Mn doped ZnS crystals have been found to have high luminescent efficiencies at room temperature [6]. ZnSe has potential for application in blue-green semiconductor lasers [7–9]. ZnTe is the binary end member of the important pseudobinary (CdZn)Te which is a commonly used substrate material for (HgCd)Te based devices. Bulk ZnTe has also been used as the sensor crystal for an electro-optic field detector [10].

Though important applications for the Zn II-VI compounds seem to be emerging, serious materials challenges remain. For example, a well-known limitation for these compounds is the inability to dope a sample either *n* or *p* to a level useful for device applications. ZnTe has been effectively doped *p* type while ZnO can be readily doped *n*. The reported maximum attainable *n* and *p* doping levels for all four Zn chalcogenide compounds varies significantly. The currently reported maximum *n* doping level decreases down the series: ZnO, ZnS, ZnSe, ZnTe. It has been suggested that vacancies and vacancy complexes contribute to carrier compensation in many of the II-VI materials [11–13]. However, the work of Laks et al. [7,14] suggests that defect concentrations in ZnSe are too low ($\sim 10^5 \text{ cm}^{-3}$ at room temperature) to act as a complete carrier limiting compensation source.

Impurity solubility/incorporation within the crystal lattice is another possible source for doping limitations. It has been proposed that donor/acceptor solubility is the primary factor determining the ultimate doping level in these materials, not compensation via defects [15]. We take that view here and use a standard model from statistical mechanics to study halogen donor incorporation. As a result, we are able to demonstrate that limitations for donor incorporation can lead to the observed trend in

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maximum n doping in the Zn chalcogenides and further that the relative efficiency of the halogens as donors can be predicted.

Consider now some of the measured and computed physical quantities of the Zn chalcogenides that show a correlation with their reported maximum attainable n type carrier concentration. Desnica [16] has shown how the ratio of covalent radii, anion/cation, is somewhat correlated with the maximum attainable p and n doping level in many of the II-VI semiconductor systems. Here we refer to the less electronegative group II member as the cation while the more electronegative group VI member is the anion. They point out that if the cation has the smaller of the two covalent radii then the material tends to be p type, while if the anion radius is the smaller of the two it can be doped n . This report encouraged us to search for other trends between maximum n carrier densities and tabulated, or easily estimated, physical properties for these compounds. We find that no fewer than six such properties have values that vary in a correlated way with the trend in maximum reported n doping level for the Zn chalcogenides. These include heats of formation, anion covalent radii, diatomic bond strengths, electronegativity differences, p - d repulsion energies and the 1 atm melting temperatures. These quantities, along with the reported maximum n doping levels, are listed in Table 1. We note that as the heat of formation increases, maximum n doping level increases. As anionic covalent radii decrease, n doping level increases. As diatomic bond strengths increase, n doping level increases. The Pauling electronegativity difference increases as n doping level increases. 1 atm melting temperatures increase as maximum n increases. Finally, estimated p - d repulsion energies increase as the maximum n doping level increases. Surely, not all six of these correlations are coincidental and we here use one of these trends within the framework of a standard model to predict the maximum donor impurity concentration.

The steps are as follows. We use the trend in diatomic bond energies to estimate a particular heat of reaction, which can then be related to a formation energy in an impurity solubility/incorporation model. A standard derivation from statistical mechanics shows that the fraction that incorporates is given by an exponential function involving the formation energy. This is a standard result used for the study of impurities in solid solutions obtained from the melt. However, the semiconductors mentioned here are typically layer grown epitaxially and even remain as thin films in the final state. Therefore, the result, obtained from the above-mentioned model, is compared to another expression for maximum donor concentration. In this expression, the maximum concentration is determined by impurity diffusion and the energetics of a depletion region at the surface. Assuming that both models are descriptive here, the two are compared and an expression is derived where the activation energy for diffusion is given in terms of the formation energy and the potential of the depletion region. The resulting diffusion activation energies are similar to others given in the literature and reveal a doping efficiency trend for the halogens, which agrees with that predicted by the computed formation energies obtained from the donor solubility/incorporation model thus demonstrating the similarity of the two models for estimating the maximum n doping level.

2. Incorporation of a donor impurity

Consider impurity doping for one of the Zn II-VI compounds mentioned above. Introduce N_D donor impurity atoms into N available sites. The driving force for incorporation is the increase in entropy relative to the pure crystal and pure donor. The total number of configurations available to the impurity donor is given by

$$\frac{N!}{N_D!(N-N_D)!} \quad (1)$$

Then, using Boltzmann's formula for the entropy, the configurational entropy increase upon mixing ΔS , can be written as

$$\Delta S = k_B \ln \left[\frac{N!}{N_D!(N-N_D)!} \right] \quad (2)$$

There is a formation energy E required for the incorporation of the donor into the lattice site. This opposes the natural drive to incorporate via entropy and leads to an equilibrium situation, i.e. the level of maximum impurity incorporation. Let the ratio of donors to available sites be $c = N_D/N$. Ignoring the change in entropy due to vibration, the classic expression for the change in free energy upon donor incorporation can be written. e.g. see Refs. [17,18].

$$\Delta G = cNE + k_B T N \left(\ln \frac{(cN)^c}{N} \right) + k_B T \ln(N - cN)^{(N-cN)} \quad (3)$$

Here Stirling's approximation has been used since both N_D and N are large, i.e. $\sim 10^{20} \text{ cm}^{-3}$. At equilibrium, $\partial \Delta G / \partial c = 0$ and, given that $E > k_B T$, Eq. (3) leads to the often used exponential expression for impurity concentration.

$$c = e^{-E/k_B T} \quad (4)$$

Reinhold and Wienecke [19] have demonstrated that substitutionally distributed donor and acceptor impurities in II-VI compounds are highly efficient. Han et al. [20] reported that nitrogen acceptors placed on substitutional sites within ZnTe are almost 100% effective. So we assume 100% ionization of shallow donors. This leads to an expression for the maximum n doping level.

$$n_{max} = Ne^{-E/k_B T} \quad (5)$$

Expressions of this type have been used to accurately describe the incorporation of impurities within a variety of materials. [21–23] and donor concentration within II-VI semiconductors [24]. The intrinsic carrier concentration is assumed to be less than 10^{15} cm^{-3} and will then be ignored.

Eq. (5) can be used to study the trend in n_{max} due to donor impurity incorporation in the Zn II-VI series. Consider the halogens, which should serve as anion substitutional donors in the Zn chalcogenides. Chlorine has been used as a donor impurity in ZnSe and ZnTe [9,25,26], whereas iodine has been used in ZnS [3]. To the best of our knowledge, a carrier concentration value has only been given for the cases of chlorine in ZnSe [9] and iodine in ZnS [3]. A difference in diatomic bond strengths can be used to estimate the formation energy, E . We next propose that doping can be

Table 1

Collected data for the cation-anion (C-A) II-VI compounds considered here. Here n_{max} is a reported maximum n doping level, ΔH_f standard state heats of formation, r_A covalent radii and E_B diatomic bond strengths (dissociation energies). ΔE_{pd} are p - d repulsion energies estimated with an expression suggested by Wei [31] using data from Wei [31] and Harrison [32]. T_m is the 1 atm melting temperature. *Refs. [36] and [37].

C-A	n_{max} (10^{20} cm^{-3})	ΔH_f (kJ/mol) [33]	r_A (pm) [34]	E_B (kJ/mol) [35]	$\chi_A - \chi_C$ [45]	ΔE_{pd} (eV)	T_m (K) [33]
ZnO	11.0 [30]	643	63	250	1.9	3.3	2250
ZnS	0.5 [3]	477	103	224, 205*	0.9	0.72	2103
ZnSe	0.15 [9]	422	116	171	0.8	0.43	1788
ZnTe	0.004 [44]	376	136	118	0.5	0.22	1568

represented as an idealized single displacement reaction involving a halogen donor impurity, and the diatomic Zn chalcogenide,



from which a heat of reaction ΔH_{rxn} can be computed. Here X is the halogen donor and A is the group VI anion. Now, the heat of reaction, ΔH_{rxn} , can be computed as

$$\Delta H_{\text{rxn}} = \sum H_{\text{prod}} - \sum H_{\text{reac}}, \quad (7)$$

where the sums are of the bonds strengths of the products and reactants. Fortunately, values for diatomic bond strengths, (dissociation energies), have been reported for the molecules involving Zn and the chalcogens and Zn with the halogens F, Br, I, and Cl. Using these data, heats of reaction are computed using Eq. (7) for each of the four Zn II-VI compounds with each of the four halogens. The results are listed in Table 2. As with the quantities listed in Table 1, these heats of reaction show a correlation with maximum n doping level.

The trend between reported maximum carrier level, n_{max} , and this ΔH_{rxn} is used to develop an estimate for the formation energy E . Though the reported values for n_{max} were obtained using a variety of donors, some non-halogens, we assume, based upon the correlation shown in Table 1 that the trend in n_{max} down the series is approximately independent of donor species. Thus, we suspect that the trend will hold with each of the halogen donors as well. Letting $N = 2.2 \times 10^{22} \text{ cm}^{-3}$, which is approximately the number of anion sites in these binary compounds [14,23,24], we plot $\ln(n_{\text{max}}/N)$ versus ΔH_{rxn} for each of the II-VI systems with each of the halogen donors. Here the temperature is set to the constant value of 800 K, chosen to be within the reported range for epitaxial growth [27]. These data points can be fitted to a straight line with the results for the case of chlorine being shown in Fig. 1. Plots of the

Table 2
Heat of reaction values (ΔH_{rxn}) in kJ/mol computed using Eq. (7). Bond dissociation energies taken from Ref. [35]. Refs. [36] and [37]. Error for the listed data is given in the cited references.

	Cl	I	Br	F
ZnO	-21.0	-97.0	-112.0	114.0
ZnS	4.2, 24.0*	-71.8, -51.9*	-86.2, -67.0*	139.2, 159.0*
ZnSe	58.3	-17.6	-32.7	193.3
ZnTe	111.4	35.4	20.4	246.4

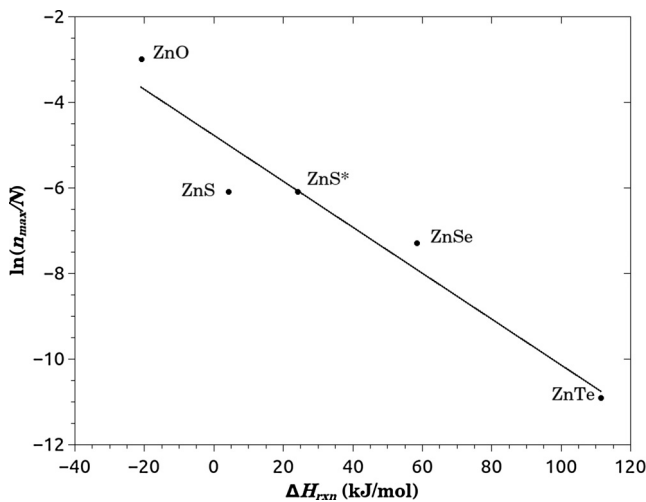


Fig. 1. Plot of heat of reactions from Table 2 vs. $\ln(n_{\text{max}}/N)$ with a linear curve fit. n_{max} values are from Table 1. The heat of reactions are for the case of Cl. Plots of the same data for the other halogens considered here yield the same slope but different intercept. Diatomic dissociation energies taken from Ref. [35]. Refs. [36] and [37]

Table 3

Formation energies for halogen donors in the Zn (II-VI) semiconductors computed using Eq. (9). α and Φ values come from curve fits as depicted in Fig. 1 and are listed in Table 4. Various other formation energies from the literature are given for comparison.

	E (eV)		
	Cl	I	Br
ZnO	0.26	0.30	0.32
ZnS	0.37	0.42	0.43
ZnSe	0.51	0.56	0.57
ZnTe	0.68	0.72	0.73
Reported formation energies:			
	0.5 eV, hypothetical for incorporation of a dopant into intrinsic material [15]		
	0.4 eV P in Si, 700–1050 °C, [22]		
	0.56 eV Sb in Si, 800 °C, [22]		
	0.38 eV N in ZnSe [24]		
	0.27 eV N in ZnTe [24]		

same data for the other halogens considered here yield the same slope but different intercept. The fit to the data shows that the line is of the form

$$\ln\left(\frac{n_{\text{max}}}{N}\right) = \frac{-\Phi}{RT} + \frac{\alpha\Delta H_{\text{rxn}}}{RT}. \quad (8)$$

Here Φ is an energy obtained from the vertical intercept and α/RT is the slope. Eq. (8) is then equivalent to Eq. (5) when

$$E = \Phi - \alpha\Delta H_{\text{rxn}}. \quad (9)$$

Accordingly, the formation energies are estimated using the results from each of the curve fits. These formation energies are listed in Table 3 along with others reported in the literature for comparison.

3. Coulombic repulsion

The compound semiconductors considered here are typically layer grown via vapor and left as thin films in the final state. Though the model considered in the previous section is quite general, one often associates it with bulk crystal growth from the melt. However, we demonstrate here that the result for n_{max} determined in the section above is related to an alternative model where the limiting factor is the electric field due to a depletion region at the growing semiconductor surface. Surface states within the energy gap can generate a depletion region, which causes the conduction band to curve upwards at the surface. This energy shift from the conduction band edge in the interior is referred to as the surface potential ϕ , [28]. The fermi level becomes pinned in the gap. This electric field in the depletion region imparts a drift velocity on donor ions in the direction of crystal growth. Schubert [27] proposed that n_{max} occurs when the magnitude of the crystal growth velocity equals the magnitude of the drift velocity. From this, he derives the equation

$$n_{\text{max}} = n_0 e^{2E_a/RT} \frac{RT}{\phi}. \quad (10)$$

Here E_a is the donor diffusion activation energy and n_0 is assumed to be a constant. Equating Eq. (5) with Eq. (10) and solving for E_a yields

$$E_a = \frac{1}{2} \left[\alpha\Delta H - \Phi - RT \ln\left(\frac{n_0 RT}{N\phi}\right) \right]. \quad (11)$$

With appropriate values for the parameters in Eq. (11), diffusion activation energies can be computed for the halogen donors within the Zn II-VI systems. Schubert used Eq. (10) to study Be doped GaAs. Using data from this work we find that $n_0 = 4.3 \times 10^{-4} \text{ cm}^{-3}$, a value which we assume is transferable when Eq. (10) is

Table 4

Diffusion activation energies for halogen donors in the Zn (II-VI) semiconductors computed using Eq. (11). α and Φ values come from curve fits as depicted in Fig. 1. φ taken from Ref. [27]. n_{\max} values used are listed in Table 1. ΔH_{rxn} values are listed in Table 2. (For ZnS, we use the average value of ΔH_{rxn} for each donor from Table 2). Various other activation energies from the literature are given for comparison. $\Phi = -0.17$ eV for F.

	E_a (eV)		
	Cl	I	Br
ZnO	2.00	1.97	1.96
ZnS	1.94	1.914	1.907
ZnSe	1.87	1.85	1.84
ZnTe	1.78	1.76	1.756
Φ (eV)	0.33	0.61	0.67

Reported activation energies:
 P bulk diffusion in CdTe: 1.99 eV Ref. [38], 2.10 eV Ref. [39]
 Na in Diamond: 1.6 eV [40]
 Te self diffusion in CdTe: 1.38 eV [41]
 Cd self diffusion in CdTe: 2.07 eV [41]
 Pb bulk diffusion in CdTe: 2.3 eV [42]
 Ge bulk diffusion in PbTe: 1.30–1.47 eV [43]

$$\alpha = -0.356$$

used to study other systems, i.e. we propose that n_{\max} is solely determined by the two energy values in Eq. (10). Values for φ for the II-VI systems studied here have to our knowledge, not been reported. However, a value of 0.9 eV has been given for Si [28] and 0.7 eV has been reported for GaAs [27]. If we let $\varphi = 0.7$ eV and use the values of $\alpha\Delta H_{\text{rxn}}$ and Φ determined previously, we are able then to compute E_a for each of the halogens as impurities within the Zn chalcogenides. These values are reported in Table 4 along with other related values from the literature for comparison.

The trends in the computed diffusion activation energies agree with that of the formation energies regarding doping efficiency of the halogens. That is, as the formation energy decreases, doping efficiency increases. As the diffusion activation energy increases donor efficiency improves. A similar trend in activation energies for Br, I and Cl has been reported for the II-VI compound CdTe [29].

4. The energy Φ

An explanation can be given for the energy Φ from Eq. (9). Van de Walle and Laks [24] let the impurity concentration in ZnSe and ZnTe be given by an expression equivalent to Eq. (5). Then, they propose a formation energy, which we here generalize for the case of the four Zn chalcogenides with each of the halogen impurity donors:

$$E = \epsilon(\text{ZnA} : \text{Ha}_A) - \mu_D + \mu_A. \quad (12)$$

In the language of Van de Walle and Laks [24], ϵ is the total energy derived from a calculation for a substitutional halogen. μ_D and μ_A are the chemical potentials for the donor and the anion respectively. On comparison with Eq. (9) we propose that $\Phi = \mu_A - \mu_D$ and that $\alpha\Delta H_{\text{rxn}} = -\epsilon$.

The model of Eq. (5) fails when $\Phi < 0$, i.e. when $\mu_A - \mu_D < 0$. This is the case for fluorine. The explanation is that the comparatively high values for the energy ϵ leads to the requirement that the chemical potential of the donor must exceed that of the anion; a situation which apparently does not favor incorporation. To our knowledge there is no report of fluorine being used successfully as a donor within these Zn II-VI systems.

5. Conclusion

Here we investigated the incorporation of donor impurities in Zn chalcogenides using a standard model from statistical mechan-

Table 5

Maximum n doping levels and dopant reported in the literature along with values for halogen donors computed using Eq. (5) with the formation energies from Table 3. References for the experimental data are given in Table 1.

	n_{\max} (10^{20} cm $^{-3}$) Eq. (5)			
	Exp	Cl	I	Br
ZnO	11 (Ga)	5.1	2.8	2.1
ZnS	0.5 (I)	1.0	0.49	0.43
ZnSe	0.15 (Cl)	0.14	0.070	0.057
ZnTe	0.004 (Al)	0.012	0.0065	0.0056

ics. Assuming 100% effectiveness of substitutional donors this leads to an expression for the maximum majority carrier concentration. Through this expression, the maximum concentration is shown to depend upon a formation energy. We were able to estimate this formation energy by using a trend between reported maximum n doping levels and a proposed heat of reaction between the diatomics of the species involved. Assuming that the trend in maximum attainable doping level down the Zn II-VI series is approximately independent of donor species we use this result to determine the effectiveness of halogen donors. Predicted maximum n doping levels for each of the halogens, Br, I and Cl in each Zn II-VI compound considered here are listed in Table 5. In two of the entries in Tables 1 and 5, namely ZnSe:Cl and ZnS:I, the value of n_{\max} has been determined experimentally. The computed values from Table 5 are essentially identical to these; well within the margin of experimental error. Results lead us to suggest that halogen substitutional impurities will serve as donors in the Zn II-VI compounds in order of increasing effectiveness as: F, Br, I, Cl, with fluorine likely being a poor candidate for incorporation at any level. Further, the results in Table 5 suggest that the maximum n doping level in ZnS and ZnTe can be increased by using Cl as the impurity donor.

As reasonable as the curve fit shown in Fig. 1 appears, some caution should be exercised. With the exception of ZnF, the errors reported for the experimental values of the diatomic dissociation energies range from a low of 6.3 kJ/mol to a high of 25.9 kJ/mol. In the case of ZnO, the dissociation energy has been assigned the maximum value consistent with the estimated error range. Nonetheless, the logical nature of the correlations derived from Eqs. (7) and (8) would seem to be immune to any major reduction in the range of the experimental error.

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