Absorption limit in direct gap III–V semiconductors

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ABSTRACT

The comparison of experimentally found absorption limits, and their variations in compound semiconductors, with theoretical expectations was never a particularly studied subject, although absorption limits in semiconductors could be critical to certain optoelectronic device applications. We introduce a model, which accurately fits the distinct absorption saturation parameter linked to the effective electron density of states.

INTRODUCTION

Despite optical properties of semiconductors have been studied for many years,[1–6] the topic is still actively addressed due to open questions regarding the exact nature of the band tailing and potential applications in such as the detailed balance in solar cells.[7] In these systems, defects and thereby many body interactions are interesting for their roles in tuning the optical absorption and corresponding limiting conditions,[7] which is why theories fitting the absorption coefficient vs the impinging photon energy, hereafter $\alpha(E)$, are a considerable part of the former and current research.[5–9] However, it was never elaborated whether the theoretical models fit quantitatively the absorption saturation. The standardized fitting routines employ phenomenological parameters to achieve satisfactory results when fitting an absorption spectrum in bulk semiconductors.[9,10] One of these parameters is "A," present in the canonical equation presented by Bardeen et al.,[11] and plays a significant role in the fitting of absorption at the saturation region. While highly effective in predicting critical material features, the physical interpretation of A was never addressed. Investigating the inherent link between A and the material properties is, thus, important. In this letter, the absorption limit in semiconductors is probed through the evolution of A as the band parameters change in different materials, such as III–V direct bandgap semiconductors.

THEORETICAL MODEL AND RESULTS

Previously, based on the modified Urbach rule,[9] we fitted $\alpha(E)$ for various semiconductors by employing the joint density of states (JDOS) expressions below:[10]

$$\alpha(E) = A\sqrt{E - E_{\mathrm{g}} + \frac{kT}{2\sigma}} \tag{1}$$

and

$$\alpha(E) = A\sqrt{\frac{kT}{2\sigma}e^{\frac{\sigma[E-E_{\mathrm{g}}]}{kT}}}, \tag{2}$$

which are valid for $\alpha(E) \geq E_{\mathrm{g}}$ and $\alpha(E) < E_{\mathrm{g}}$, respectively, whereas A is considered as a fitting constant without further interpretation, E_{g} is the optical bandgap, kT (=0.025 eV) is the thermal energy at room temperature (RT), and σ is a parameter defining the steepness of the Urbach tail absorption and, therefore, is a measure for the purity and disorders of semiconductors.[12] However, Eq. (2), which represents the modified Urbach rule, shows that σ and A are inherently linked, i.e., the value of A reflects the purity of the material as well.

In the following, we compare A found from fits of experimental results with the theoretically expected values, denoted hereafter with A^*. The expression for the latter was pointed out by Bardeen et al.,[11]

$$A^* = \left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{(2(m_{\mathrm{e}}^* m_{\mathrm{h}}^* / m_{\mathrm{e}}^* + m_{\mathrm{h}}^*))^{3/2}}{\pi n c m_{\mathrm{e}}^* \hbar^2}, \tag{3}$$

where e is the elementary charge, ε_0 is the permittivity of the vacuum, m_{e}^* and m_{h}^* are the effective mass of the electron and hole,
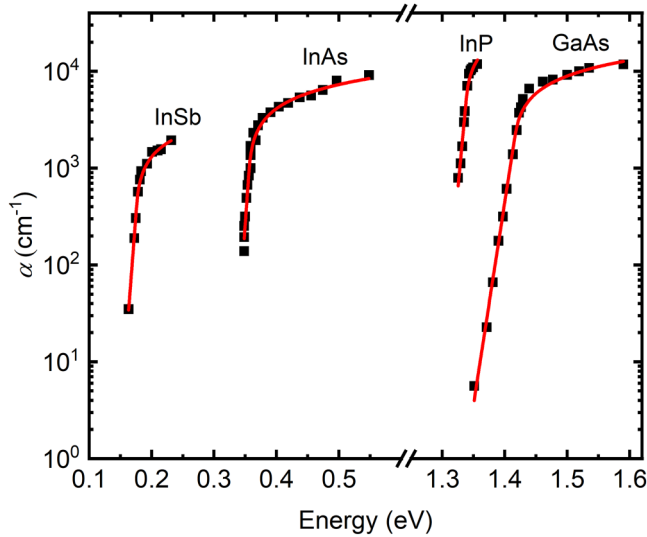
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FIG. 1. $\alpha(E)$ measurements (symbols) adapted from Ref. 10, and the corresponding fits (lines) calculated with Eqs. (1) and (2).
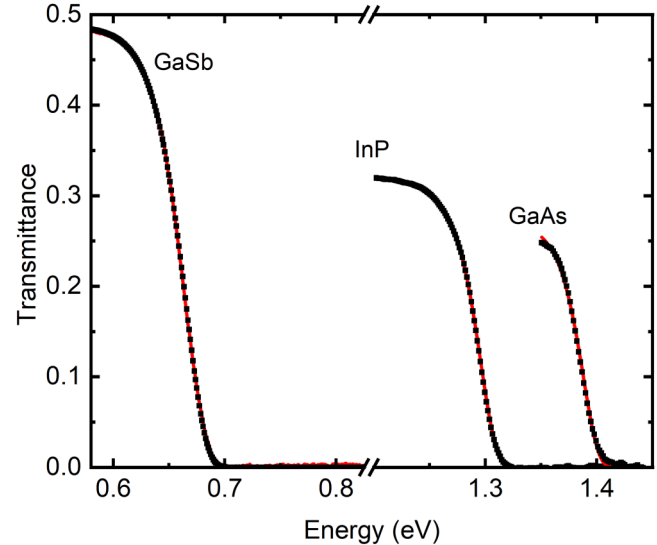

FIG. 2. Tr(E) measurements (symbols) and corresponding fits (lines) using Eqs. (1)–(3).

respectively, n is the refractive index in the vicinity of E_g, c is the speed of light, and $\hbar$ is the reduced Planck constant. With the fine structure constant,

$$\alpha_f = \left(\frac{e^2}{4\pi\varepsilon_0}\right)\frac{1}{c\hbar} = \frac{1}{137}, \qquad (4)$$

and the reduced effective mass,

$$m_r^* = \frac{m_e^* m_h^*}{m_e^* + m_h^*}, \qquad (5)$$

Eq. (3) takes the form

$$A^* = 2\alpha\frac{(2m_r^*)^{3/2}}{n m_e^* h}. \qquad (6)$$

Figure 1 summarizes fits of $\alpha(E)$ at RT for InP, InAs, InSb, and GaAs from our former work (Ref. 10), and Table I shows the corresponding fit parameters used in Eqs. (1) and (2). The symbols are the experimental data retrieved from the literature, while the lines represent the fits. Table I also depicts the material parameters used to calculate A^*. All material related parameters used herein were retrieved from Refs. 4 and 13. Within a factor of 2, we found good agreements between A and A^* values, apart from InP, i.e., 9×10^4 vs 1.6×10^4 cm^{-1} eV$^{-1/2}$, respectively. However, we noticed that the uncertainty of A is the largest for the InP fit and concluded that the limited data points (particularly above E_g) are the reason for the increased uncertainty, and the discrepancy between A and A^*. Therefore, using a Perkin Elmer Lambda 95 spectrometer, we performed transmittance (Tr) measurements at RT on an InP wafer to get a more accurate A value. Additionally, to confirm the harmony of both fitting procedures, we measured Tr of GaAs and GaSb wafers. The Tr(E) spectra are fitted as described in Ref. 14

TABLE I. Material and fit parameters to fit $\alpha(E)$ in Fig. 1 with Eqs. (1) and (2) and to calculate A^*.

	InP	InAs	InSb	GaAs
A (cm^{-1} eV$^{-1/2}$)	$9 \times 10^4 \pm 7560$	$1.9080 \times 10^4 \pm 1488$	$8 \times 10^3 \pm 416$	$3 \times 10^4 \pm 3360$
E_g (eV)	1.338 ± 0.002	0.356 ± 0.003	0.176 ± 0.001	1.416 ± 0.004
σ	3.96 ± 0.36	5.255 ± 0.851	4.885 ± 0.303	2.408 ± 0.130
n	3.37	3.42	3.75	3.40
m_e^*/m_0	0.067	0.022	0.014	0.068
m_h^*/m_0	0.8	0.41	0.40	0.5
m_r^*/m_0	0.062	0.021	0.014	0.060
A^* (cm^{-1} eV$^{-1/2}$)	1.6×10^4	9.6×10^3	7.5×10^3	1.5×10^4

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TABLE II. Fit parameters obtained from Tr(E) fits in Fig. 2, using Eqs. (1), (2), and (7).

	InP	GaAs
A (cm^{-1} eV$^{-1/2}$)	$1.35 \times 10^4 \pm 355$	$1.485 \times 10^4 \pm 666$
E_g (eV)	1.338 ± 0.002	1.429 ± 0.003
σ	1.80 ± 0.014	1.926 ± 0.223
C	0.312 ± 0.08	0.267 ± 0.03

using Eqs. (1) and (2) and

$$\text{Tr}(E) = Ce^{-\alpha(E)d}, \tag{7}$$

where C is a scaling constant factoring in mostly the reflection and d (=300 μm) is the thickness of the wafers investigated. The measured Tr(E) spectra (symbols) and their fits (solid lines) are shown in Fig. 2. The equivalent results to Table I, using the Tr data for InP, GaAs, and GaSb, are displayed in Tables II and III, respectively. Indeed, with the increased number of data points provided by the InP $Tr(E)$ spectrum, the fit result $A = 1.35 \times 10^4$ cm^{-1} eV$^{-1/2}$ closely matches $A^* = 1.6 \times 10^4$ cm^{-1} eV$^{-1/2}$, while the A value for GaAs in Tables I and II is in very good harmony as well.
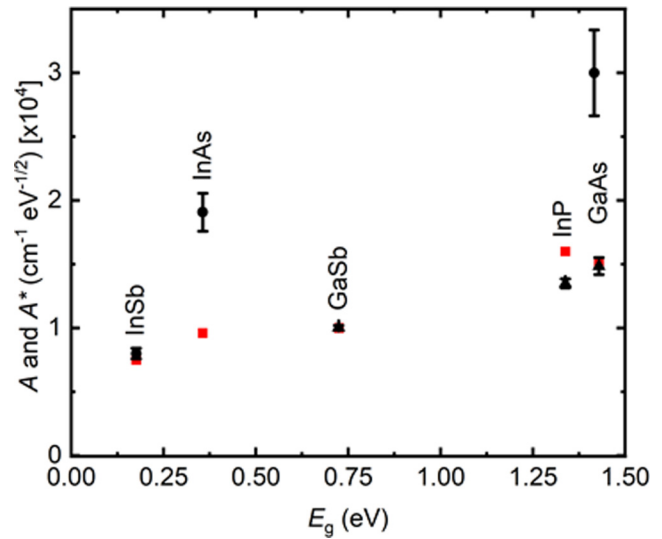
DISCUSSION AND CONCLUSION

Figure 3 visibly emphasizes the good agreement of A and A^* in Tables I–III. The square symbols represent A^*, whereas the round and triangle symbols represent A stemming from the fits of $\alpha(E)$ and Tr(E), respectively, while the flyer of the A value for InP in Table I is omitted. Figure 4 shows the linear fits of A^* and m_r^*/m_0 vs E_g represented by a broken and solid line, respectively. The fits demonstrate that the semiconductors become more and more opaque with increasing bandgaps because of the growth of the effective electron density of states with enlarging E_g.[15]

The good agreement between A and A^* not only validates the fitting model but also provides a guide to the limiting values the parameters could take. The variation of A could possibly be linked to the degree of disorder in the system and could be investigated in greater detail if measurements from the samples of same specimen with varied degrees of impurities or strains in them are compared.

TABLE III. Material and fit parameters to fit Tr(E) of GaSb in Fig. 2 with Eqs. (1), (2), and (7) and to calculate A^*.

	GaSb
A (cm^{-1} eV$^{-1/2}$)	$1.003 \times 10^4 \pm 166$
E_g (eV)	0.724 ± 0.001
σ	1.427 ± 0.005
C	0.487 ± 0.003
n	3.90
m_e^*/m_0	0.047
m_h^*/m_0	0.23
m_r^*/m_0	0.039
A^* (cm^{-1} eV$^{-1/2}$)	1.0×10^4

FIG. 3. The comparison of A and A^* values from Tables I–III. The square symbols represent A^*, whereas the round and triangle symbols represent A stemming from the fits of $\alpha(E)$ and Tr(E), respectively.

In applications, such as solar cells and light emitting devices, it is critical to assess the detailed balance between absorption and emission. In several different geometries of photovoltaic devices over the last few decades, the principle of detailed balance has been demonstrated.[7] The work shows that the absorption limit in bulk semiconductors can be a pathway for understanding the detailed balance in systems, which are more complex in structure and geometries. The framework of analysis presented is simple, flexible,
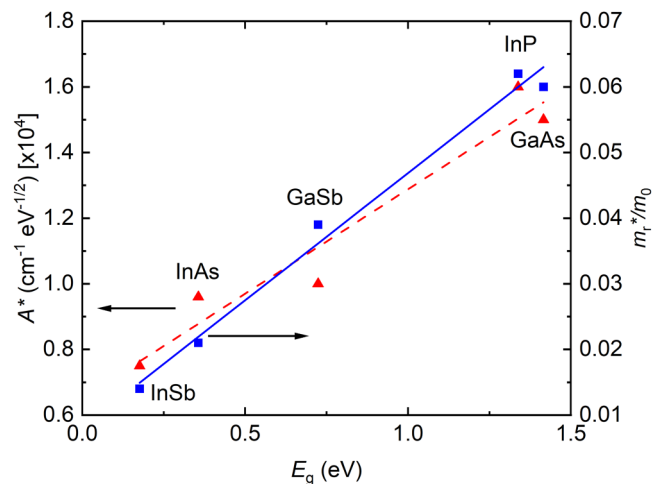
FIG. 4. Trend of A^* (broken line) and m_r^*/m_0 (solid line) vs E_g of the semiconductors investigated.

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yet powerful enough to extract material parameters from either absorption or Tr measurements using a consistent model based on the JDOS represented by Eqs. (1) and (2).

To summarize, absorption limits in five bulk, III–V direct gap semiconductors were investigated using $\alpha(E)$ data from the literature and our Tr experiments. We demonstrated good agreement between A and A^*, while the work particularly stresses that Tr measurements, even when performed through wafers with a thickness of $300\,\mu$m, are an accurate method to determine the absorption limit of semiconductors at RT, where excitonic effects are for the most part negligible.

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AUTHOR DECLARATIONS

Conflict of Interest

The authors have no conflicts to disclose.

Author Contributions

Mithun Bhowmick: Formal analysis (equal); Investigation (lead); Methodology (equal); Resources (lead); Software (lead); Visualization (lead); Writing – original draft (equal); Writing – review & editing (lead). **Haowen Xi:** Formal analysis (equal); Methodology (equal). **Bruno Ullrich:** Conceptualization (lead); Formal analysis (lead); Investigation (equal); Methodology (equal); Visualization (equal); Writing – original draft (lead); Writing – review & editing (equal).

DATA AVAILABILITY

The data that support the findings of this study are available within the article.

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