PHYSICAL REVIEW B **106**, 214102 (2022)

Overcoming the doping limit in semiconductors via illumination

Xuefen Cai,[1] Jun-Wei Luo,[1,2] Shu-Shen Li,[1,2] Su-Huai Wei,[3,*] and Hui-Xiong Deng[1,2,†]
[1] *State Key Laboratory of Superlattices and Microstructures, Institute of Semiconductors, Chinese Academy of Sciences, Beijing 100083, China*
[2] *Center of Materials Science and Optoelectronics Engineering, University of Chinese Academy of Sciences, Beijing 100049, China*
[3] *Beijing Computational Science Research Center, Beijing 100193, China*

(Received 17 July 2022; revised 19 November 2022; accepted 22 November 2022; published 5 December 2022)

It has been shown that illumination could have significant effects on the dopability in semiconductors. However, a general understanding on these effects is still lacking. In this paper, we present a self-consistent scheme to study the doping properties in semiconductors under illumination, and unravel a general picture: the excess carriers induced by illumination can substantially suppress the formation of compensating defects and enhance the carrier mobility as well as the density of the majority carrier, because the illumination leads to an asymmetric Fermi level shift. This is exemplified by a prototype Mg doped GaN system upon exposure to light and is consistent with available experimental observations. Our work provides a fundamental understanding of the physical process occurring in semiconductors upon illumination, and paves the way to overcome the doping bottleneck via nonequilibrium techniques in semiconductors.

DOI: 10.1103/PhysRevB.106.214102

I. INTRODUCTION

Doping in semiconductors plays a decisive role in modern electronics and optoelectronics [1–3]. Low solubility of dopants, deep ionization energy level, and spontaneous formation of compensating defects are the three major factors that limit the dopability in a semiconductor. The former two obstacles are closely linked to the dopant species and growth conditions, which could sometimes be overcome via properly choosing growth conditions and doping species, while the latter one is an intrinsic problem and has been always very difficult to overcome under thermodynamic equilibrium conditions [4,5].

Defect formation energy is the critical quantity characterizing the degree of difficulty in forming a defect. As schematically depicted in Fig. 1(a), the formation energies of charged acceptor A^- (donor D^+) increases (decreases) linearly as the Fermi level decreases. Assuming one intends to dope a semiconductor p type, the incorporation of hole-producing acceptor shifts the Fermi level toward the valence band maximum (VBM), increasing (decreasing) the formation energy of A^- (D^+), thus favoring the formation of hole-killing compensating donor and finally pinning the equilibrium Fermi level deep within the band gap at E_{F0} and negating further progress in the p-type doping. As such, it is almost impossible to simultaneously achieve high doping efficiency and reduce compensation under the equilibrium growth condition in a system characterized by a single Fermi level for both electrons and holes.

However, under some nonequilibrium growth conditions, it may be possible to decouple the Fermi levels for electrons and holes. Experimentally, it was observed that illumination during growth could enhance the doping efficiency for several compounds such as CdTe, GaN, and ZnX (X = O, S, Se, Te) [6–12]. While several computational schemes have been proposed in the past to study the illumination effects on the dopability in semiconductors, a general understanding on these effects is still lacking. We recognize a set of facts as follows: (i) It is still under debate whether the increase of carrier density is originated from the increase in the concentration of target dopants [8] or reduction in the concentration of compensating native defects [12–15], if not both [16]. (ii) The existing computational schemes are incomplete and have some limitations. For instance, the studies in Refs. [15,16] do not simultaneously consider the charge balance, as well as the balance between generation and recombination of carriers. More importantly, (iii) the discussions of the illumination effect are based on specific compounds [15,16] and/or simplified model systems [13] rather than on the general perspective abstracted from the basic concepts, so the universality and validity of the prior drawn conclusions are in doubt.

In this work, we first develop an analytic and universal scheme for characterizing the doping properties in semiconductors under steady-state illumination. Based on the derivation of the carrier density formula, we show that the variation of Fermi level is inversely proportional to the carrier concentration. Therefore, the excess carriers induced by illumination leads to an asymmetric shift of the effective Fermi levels for electrons and holes, yielding a negligible decrease in the concentration of target defects as compared to that of compensating defects. As such, we found that the illumination can drastically increase the majority-carrier concentration

---

[*] suhuaiwei@csrc.ac.cn
[†] hxdeng@semi.ac.cn

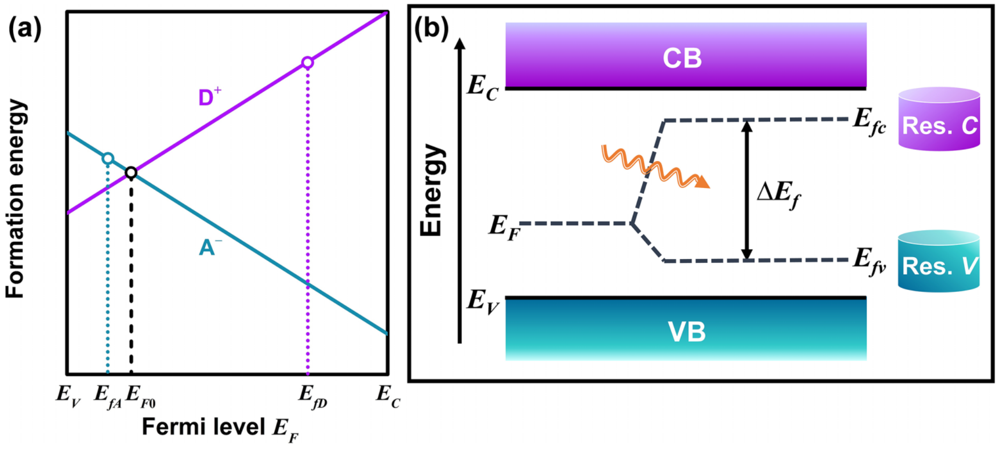

FIG. 1. (a) Schematic plot of the dependence of defect formation energy on the Fermi level for a *p*-type semiconductor with a hole-producing acceptor *A* and a hole-killing donor *D*. (b) Energy diagram of a semiconductor going from equilibrium to nonequilibrium steady state condition under illumination (wavy arrow). In this case, the equilibrium Fermi level (E_F) is split into two quasi-Fermi levels (E_{fc} and E_{fv}), which could be treated as two Fermi reservoirs. The band edge states (E_C and E_V) and the splitting of the two quasi-Fermi levels (ΔE_f) are also indicated.

by decreasing the concentration of compensating defects and improve the carrier mobility, consistent with previous experimental observations [6–12,17]. Next, as an example, we study the illumination effects on the doping behaviors in Mg doped wurtzite GaN (GaN:Mg) using our computational scheme to illustrate the validity of our model. The fundamental understanding developed here offers a general and feasible strategy to overcome the doping limit in semiconductors via nonequilibrium techniques.

II. RESULTS AND DISCUSSION

A. Two-Fermi-reservoir (TFR) model

The Fermi level E_F is at the heart of accessing the defect properties of semiconductors in equilibrium. Once the Fermi level is determined by solving self-consistently the implicit charge neutrality equation, one can get the electron, hole, and defect concentrations at temperature T as follows:

$$n = N_C \exp\left(\frac{E_F - E_C}{kT}\right), \tag{1}$$

$$p = N_V \exp\left(\frac{E_V - E_F}{kT}\right), \tag{2}$$

$$c(\alpha, q) = N_S \exp\left(-\frac{\Delta H_f(\alpha, q)}{kT}\right). \tag{3}$$

Here, k is the Boltzmann constant, E_C and E_V are the energies of conduction band minimum (CBM) and VBM, N_C and N_V are the effective density of states in the conduction and valence bands, respectively, and N_S is the number of possible defect sites per unit volume. $\Delta H_f(\alpha, q)$ is the formation energy of defect α in charge state q, which is generally written as a function of E_F [18,19],

$$\Delta H_f(\alpha, q) = E(\alpha, q) - E(\text{host}) + \sum n_i(\mu_i + E_i) + q(E_F + E_V) + \Delta E_{\text{corr}}, \tag{4}$$

where $E(\alpha, q)$ and $E(\text{host})$ are the total energies of the doped and undoped host with the same supercell, μ_i is the chemical potential of atom i with respect to the corresponding ground-state energy of elemental forms E_i, and n_i is the number of constituents i removed from the host cell in forming the defect cell. The ΔE_{corr} is a correction term to address the supercell finite-size effects.

When the semiconductor is exposed to illumination, as sketched in Fig. 1(b), the equilibrium Fermi level splits into two quasi-Fermi levels. It is clear from Eqs. (1) and (2) that the Fermi level shifting is $|dE_F| = \frac{kT}{N} dN$ ($N = n$ or p). That is, the shift of the Fermi level is inversely proportional to the carrier concentration N. For a p-type semiconductor, with a given amount of carrier variation $\delta n = \delta p$ generated by illumination, the shift of the hole quasi-Fermi level from the equilibrium Fermi level E_{F0} will be much smaller than the shift of the electron quasi-Fermi level from E_{F0}, because the majority hole concentration is much larger than the minority electron concentration. Similar conclusions can also be drawn for the n-type doped semiconductors, i.e., the Fermi level shift for the one associated with the majority carrier is much less than the one for the minority carrier.

The classical analogy between the equilibrium Fermi level and Fermi reservoir implies that the two quasi-Fermi levels correspond to two quasireservoirs. The quasi-Fermi levels (reservoirs) close to the CBM and VBM are denoted as E_{fc} (Res. C) and E_{fv} (Res. V), respectively. Physically, both of the quasi-reservoirs should contribute to the excitation of electrons to the conduction band and holes to the valence band. The weight that E_{fc} has on the excitation of electrons to the conduction band can be expressed as

$$w_C(E_{fc}) = \frac{\exp\left(\frac{E_{fc}-E_C}{kT}\right)}{\exp\left(\frac{E_{fc}-E_C}{kT}\right) + \exp\left(\frac{E_{fv}-E_C}{kT}\right)} = \frac{1}{1 + \exp(-\Delta E_f/kT)}, \tag{5}$$

where $\Delta E_f = E_{fc} - E_{fv}$ is the quasi-Fermi level splitting that is a proper measure of the degree that the system is out of equilibrium. Similarly, the weight that E_{fv} has on the excitation of holes to the valence band is

$$w_V(E_{fv}) = \frac{\exp\left(\frac{E_V - E_{fv}}{kT}\right)}{\exp\left(\frac{E_V - E_{fv}}{kT}\right) + \exp\left(\frac{E_V - E_{fc}}{kT}\right)} = \frac{1}{1 + \exp(-\Delta E_f/kT)}. \tag{6}$$

In this sense, we can simply introduce a weight factor

$$w = \frac{1}{1 + \exp(-\Delta E_f/kT)}. \tag{7}$$

Then, the carrier densities excited from the two reservoirs can be described by

$$n = N_C\left[w \exp\left(\frac{E_{fc} - E_C}{kT}\right) + (1 - w)\exp\left(\frac{E_{fv} - E_C}{kT}\right)\right], \tag{8}$$

$$p = N_V\left[w \exp\left(\frac{E_V - E_{fv}}{kT}\right) + (1 - w)\exp\left(\frac{E_V - E_{fc}}{kT}\right)\right]. \tag{9}$$

Note that, at equilibrium, $E_{fc} = E_{fv} = E_F$ (*i.e.*, $\Delta E_f = 0$), the weight parameter w is equal to 1/2, thus Eqs. (8) and (9) naturally go back to the equilibrium forms of Eqs. (1) and (2) [20]. If the illumination intensity is very high, it enables $\Delta E_f \gg kT$, and the weight parameter w is approaching 1, indicating that the density of electron (hole) is governed by the corresponding quasi-Fermi level E_{fc} (E_{fv}). These extreme cases manifest that the analytical forms are effective in retaining the physical significance of the system.

Likewise, the effective Fermi levels for donors (E_{fD}) and acceptors (E_{fA}) can be respectively written as

$$E_{fD} = wE_{fc} + (1 - w)E_{fv}, \tag{10}$$

$$E_{fA} = wE_{fv} + (1 - w)E_{fc}. \tag{11}$$

The formation energies of donor and acceptor under the nonequilibrium steady state can now be recast by substituting E_F in Eq. (4) with E_{fD} and E_{fA}, respectively. As such, the corresponding concentration of defect $c(\alpha, q)$ can be determined via the Boltzmann relation in Eq. (3).

Under the nonequilibrium steady state condition, the overall charge neutrality relation remains, that is,

$$\sum_{\alpha,q} q * c(\alpha, q) + p - n = 0. \tag{12}$$

Meanwhile, the generated and recombined number of carriers per unit area and per unit time must be equal. Assuming the photogeneration rate of electrons and holes is G, we get

$$G - R_{\text{BB}} - R_{\text{Aug}} - \sum_{\alpha,q} R_{\text{SRH}}(\alpha, q) = 0, \tag{13}$$

where R_{BB}, R_{Aug}, and R_{SRH} are the band-to-band [21], Auger [21], and defect-assisted Shockley-Read-Hall [22] recombination rates, respectively. They can be respectively given by

$$R_{\text{BB}} = B\gamma,\ R_{\text{Aug}} = (A_n n + A_p p)\gamma, \tag{14}$$

$$R_{\text{SRH}}(\alpha, q) = \frac{\gamma * c(\alpha, q)}{(n + n_t)/c_p + (p + p_t)/c_n}, \tag{15}$$

in which, $\gamma = (np - n_i^2)$, $c_n = \sigma_n v_{th}$, $c_p = \sigma_p v_{th}$, and $v_{th}^2 = 3kT/m^*$. n_t and p_t are the electron and hole concentrations when the Fermi level coincides with the trap level. B, $A_n(A_p)$, $c_n(c_p)$, $\sigma_n(\sigma_p)$, and v_{th} denote the rate of radiative capture probability, Auger coefficients of electrons (holes), capture coefficients of electrons (holes), capture cross section of electrons (holes), and average thermal velocity of electrons or holes, respectively. The radiative capture probability can be obtained by $B = 1/\tau(n_0 + p_0 + \Delta n)$ [21], where τ is the radiative lifetime, n_0 (p_0) is the electron (hole) density in equilibrium, and Δn is the excess electron density. These parameters can be obtained from available experimental and empirical data. Solving Eqs. (12) and (13) simultaneously and self-consistently, the values for E_{fc} and E_{fv} can be determined, then other physical parameters that describe the system, including the carrier density, defect formation energy, and defect concentration, can be readily obtained.

Building upon this two-Fermi-reservoir (TFR) model, we clarified the fundamental mechanisms of how the illumination overcomes the doping bottleneck in semiconductors. Taking a p-type semiconductor as an example, analogous to the afore stated asymmetric shifting feature between E_{fc} and E_{fv}, the effective Fermi levels for donor (E_{fD}) and acceptor (E_{fA}) also shift toward the CBM and VBM states, respectively, with the former acting much more pronounced than the latter, as shown schematically in Fig. 1(a). As a result, although the concentration of the targeted acceptor and compensating native donor are both reduced, the decrease of the compensating donor is much larger than that of the acceptor due to the much larger shift of E_{fD} compared with E_{fA}. Subsequently, the free hole concentration in the system increases, indicating that illumination during growth can improve the doping efficiency in the p-type doped semiconductors. Similar results are also predicted for n-type doped systems. Besides, given the carrier mobility $\mu = e\tau/m^*$, where τ is the scattering time and inversely proportional to the number of scatters per unit volume, the decreasing concentration of both defects can also lead to an increase in the carrier mobility at constant temperature [17,23]. Albeit the specific details vary from material to material, the above analysis and insights for the impact of illumination on the defect control in semiconductors are universal (i.e., material independent).

B. GaN:Mg system under illumination

To substantiate our main theoretical analysis above, we take Mg doped wurtzite GaN as an example. It is reported that V_{N} is the main compensating center for acceptor Mg_{Ga} in GaN [24–27]. Figure 2 depicts the calculated formation energies of Mg_{Ga} and V_{N} in GaN as a function of the Fermi level under the Ga-rich condition, which is the common experimental growth condition for GaN [28–30]. The calculations are conducted using the Projector augmented wave (PAW) method and the HSE06 hybrid density functional [31] as implemented in the

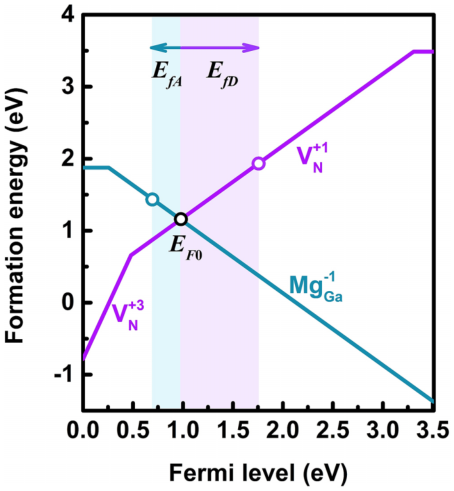

FIG. 2. Calculated formation energies ΔH_f of $\mathrm{Mg_{Ga}}$ and V_N in wurtzite GaN under Ga-rich condition as a function of the Fermi level. The zero of the Fermi level corresponds to the VBM of GaN. The E_{F0} denotes the equilibrium Fermi level (pinned at ~ 0.98 eV). The shaded areas schematically show the possible tunning range for the effective Fermi level of acceptor (cyan) and donor (lilac) in nonequilibrium steady state condition.

VASP package [32]. We set the Hartree-Fock exchange mixing parameter α to 0.31 and a cutoff energy to 520 eV for the plane-wave basis set. We construct a 96-atom supercell and employ the spin-polarized calculations for the defect system with unpaired electrons. The defect formation energy and transition energy levels are calculated as described in the literature [18,19].

$\mathrm{Mg_{Ga}}$ has a (0/–1) transition energy level around $\sim$ 0.26 eV above the VBM, while $(+1/0)$ and $(+3/+1)$ transition energy levels of V_N occur at approximately 3.3 and 0.48 eV above the VBM, respectively. These obtained defect levels are in good agreement with previous reported data [33–35]. The equilibrium Femi level is pinned at the position ($E_{F0} \sim 0.98$ eV) at which the formation energies of $\mathrm{Mg_{Ga}}$ and V_N are equal, which is far away from the VBM and unfavorable for p-type doping. The formation energy of $\mathrm{Mg_{Ga}}$ is higher (lower) than that of $\mathrm{V_N}$ when the Fermi level lies below (above) E_{F0}.

When the GaN:Mg system is uniformly illuminated with photogeneration rate G of electron-hole pairs per unit volume in the range from 1×10^{18} to 5×10^{25} $\mathrm{cm^{-3}\ s^{-1}}$, excess carrier concentrations of approximately 10^{10}–10^{17} $\mathrm{cm^{-3}}$ are expected to be generated assuming a carrier lifetime of 10 ns [36]. A common experimental growth temperature of 1000 °C is chosen herein [37]. We use the experimental electron and hole effective masses of $0.2m_0$ and $1.5m_0$ [38], respectively, for the calculations. The capture cross section of electrons (holes) for $\mathrm{Mg_{Ga}^{-1}}$ is set to 10^{-18} $\mathrm{cm^2}$ (10^{-15} $\mathrm{cm^2}$), while that for V_N^{+1} is 10^{-15} $\mathrm{cm^2}$ (10^{-18} $\mathrm{cm^2}$), and the Auger coefficients of electrons and holes are both set to 10^{-31} $\mathrm{cm^6/s}$ [39].

As expected, the two quasi-Fermi levels E_{fc} and E_{fv} get closer to the CBM and VBM of GaN with the increase of photogeneration rate G, respectively, which results in the increase of quasi-Fermi level splitting ΔE_f, as shown in Fig. 3(a). The large (small) deviation ratio of the electron (hole) density upon illumination in this p-type GaN results in a large (small) shift of the quasi-Fermi level E_{fc} (E_{fv}). Analogous to the trend of carrier quasi-Fermi level, the E_{fD} and E_{fA} also shift to the CBM and VBM of GaN as defined by Eqs. (10) and (11), respectively, and the deviation of E_{fD} is much larger than that of E_{fA}. It is thus confirmed that (i) the formation energies of the ionized defects $\mathrm{Mg_{Ga}^{-1}}$ and $\mathrm{V_N^{+1}}$ in p-type GaN both increase with the illumination (Fig. 2), leading to the reduced concentrations of these defects; (ii) the decrease of the concentration of compensating center V_N is much more significant than that of the acceptor $\mathrm{Mg_{Ga}}$ at each G, as shown in Fig. 3(b).

The calculated concentrations of both electron and hole in GaN:Mg are increased with increasing photogeneration rate G, in accord with both physical intuitions and previous experiments that the increase of illumination intensity gives rise to an increase of the densities of free carriers [12]. Specifically, the calculated increment of concentrations for electron ($\Delta\ n$) and hole ($\Delta\ p$) at G of 10^{22} $\mathrm{cm^{-3}\ s^{-1}}$ is about 4.1×10^{13} $\mathrm{cm^{-3}\ s^{-1}}$ and 1.9×10^{17} $\mathrm{cm^{-3}\ s^{-1}}$, respectively, which gives a good fit to the experimental results of $\Delta n \sim 10^{12}$–10^{14} $\mathrm{cm^{-3}}$ and $\Delta p \sim 10^{17}$ $\mathrm{cm^{-3}}$ under the similar nonequilibrium illumination condition [12].

To have practical application, it is important to know whether the photoinduced effects persist after turning off the illumination after the growth. To address this issue, we perform a self-consistent calculation in which the density of defects is frozen to the value just before the light is turned off. We find that when the illumination is turned off, the system that has been subjected to higher intensity of illumination also has a larger increment of the hole density relative to the one without illumination. For G in the order of 10^{23} $\mathrm{cm^{-3}\ s^{-1}}$, the hole density increased by nearly one order of magnitude compared to the one that has not been illuminated ($p_0 = 5.3 \times 10^{16}$ $\mathrm{cm^{-3}\ s^{-1}}$), suggesting that the illumination during growth is an effective way to facilitate the p-type doping in GaN. However, if the light intensity is extremely high, exceeding 10^{24} $\mathrm{cm^{-3}\ s^{-1}}$, a negative effect occurs, and the hole concentration starts to decrease after the light source is removed. This is because under very high light intensity, the effect of the reduced acceptor density becomes dominant compared to that of the reduced compensating donor defect.

III. CONCLUSION

To conclude, we developed a self-consistent TFR model for studying the defect properties under steady-state illumination. It is demonstrated that the illumination reduces both the concentrations of target dopants and compensating defects, but the reduction is much more pronounced in the latter, leading to net increases of carrier density as well as carrier mobility, thus enhancing the doping efficiency in semiconductors. This overall picture falls in line with the experimental observations, and has been exemplified by a Mg doped GaN system. The insights developed here not only unravel the physical mechanism of the illumination-assisted enhancement of doping efficiency, but also provide a general path toward overcoming the doping limit in semiconductors through illumination.

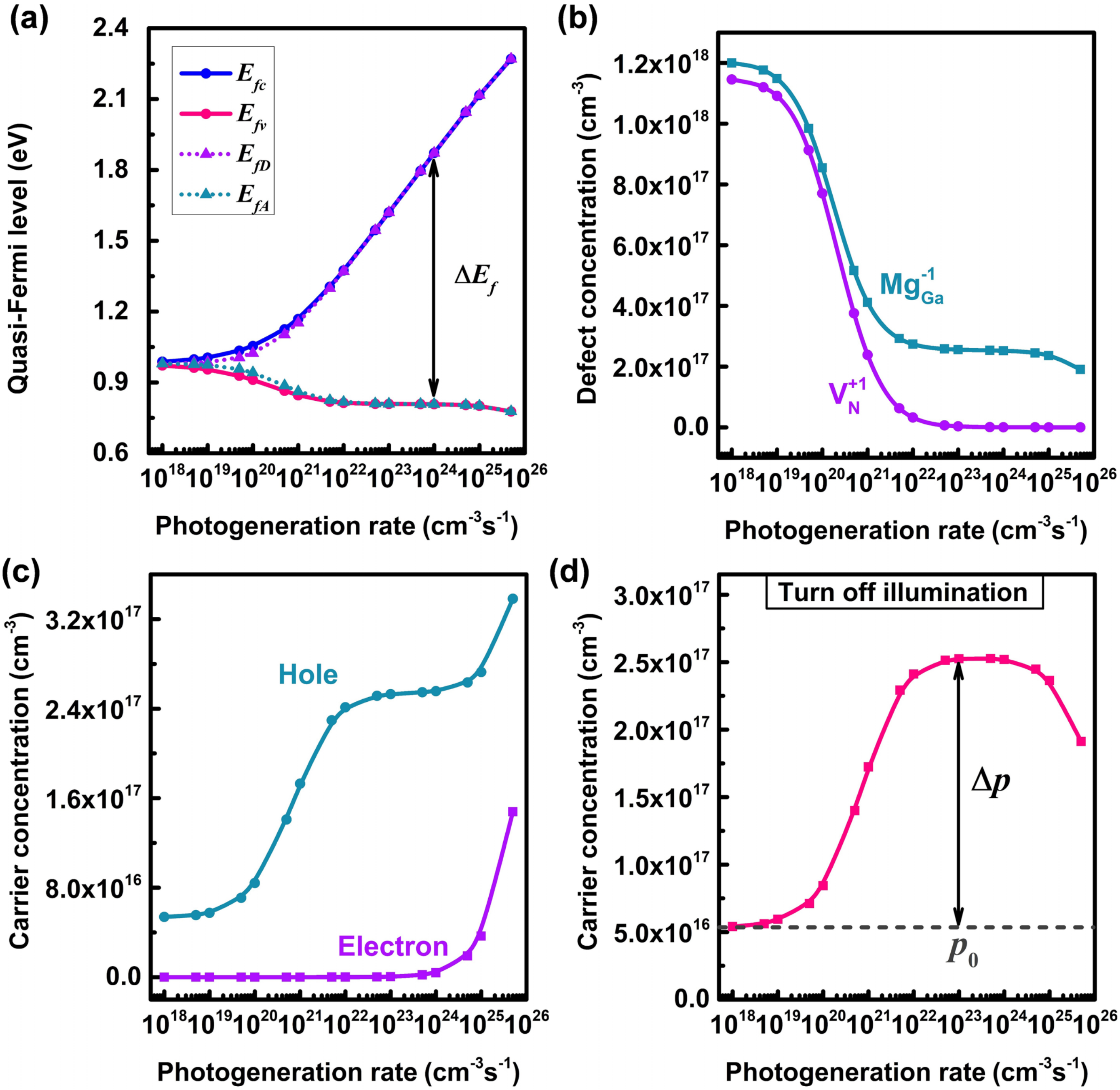

FIG. 3. (a) Two quasi-Fermi levels and two effective Fermi levels, (b) concentrations of charged defects $\mathrm{Mg}_{\mathrm{Ga}}^{-1}$ and $\mathrm{V}_{\mathrm{N}}^{+1}$, and (c) carrier concentrations in GaN as a function of the photogeneration rate G (using a logarithmic axis). (d) The postillumination hole concentration as a function of the removed G (using a logarithmic axis). The hole concentration in the dark condition p_0 is also indicated using the grey dashed line.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China (Grants No. 11991060, No. 12088101, No. U1930402, No. 61927901, No. 61922077, and No. 11874347), the National Key Research and Development Program of China (Grant No. 2018YFB2200100), the Key Research Program of the Chinese Academy of Sciences (Grant No. XDPB22), and the CAS Project for Young Scientists in Basic Research (Grant No. YSBR-026). H.-X.D. was also supported by the Youth Innovation Promotion Association of Chinese Academy of Sciences (Grant No. Y2021042). We acknowledge computational resources from the Beijing Computational Science Research Center.

[1] A. Tsukazaki, A. Ohtomo, T. Onuma, M. Ohtani, T. Makino, M. Sumiya, K. Ohtani, S. F. Chichibu, S. Fuke, Y. Segawa, H. Ohno, H. Koinuma, and M. Kawasaki, Nat. Mater. **4**, 42 (2005).

[2] Y. Taniyasu, M. Kasu, and T. Makimoto, Nature (London) **441**, 325 (2006).

[3] S. Pimputkar, J. S. Speck, S. P. DenBaars, and S. Nakamura, Nat. Photonics **3**, 180 (2009).

[4] S. B. Zhang, S. H. Wei, and A. Zunger, Physica B (Amsterdam, Neth.) **273**, 976 (1999).

[5] S.-H. Wei, Comput. Mater. Sci. **30**, 337 (2004).

[6] R. L. Harper Jr, S. Hwang, N. C. Giles, J. F. Schetzina, D. L. Dreifus, and T. H. Myers, Appl. Phys. Lett. **54**, 170 (1989).

[7] S. Fujita and S. Fujita, J. Cryst. Growth **117**, 67 (1992).

[8] J. Simpson, I. Hauksson, S. Y. Wang, H. Stewart, K. A. Prior, and B. C. Cavenett, Physica B (Amsterdam, Neth.) **185**, 164 (1993).

[9] X. Li, B. Zhang, H. Zhu, X. Dong, X. Xia, Y. Cui, K. Huang, and G. Du, Appl. Surf. Sci. **254**, 2081 (2008).

[10] Z. Bryan, M. Hoffmann, J. Tweedie, R. Kirste, G. Callsen, I. Bryan, A. Rice, M. Bobea, S. Mita, J. Xie, Z. Sitar, and R. Collazo, J. Electron. Mater. **42**, 815 (2013).

[11] Z. Bryan, I. Bryan, B. E. Gaddy, P. Reddy, L. Hussey, M. Bobea, W. Guo, M. Hoffmann, R. Kirste, J. Tweedie, M. Gerhold, D. L. Irving, Z. Sitar, and R. Collazo, Appl. Phys. Lett. **105**, 222101 (2014).

[12] A. Klump, M. P. Hoffmann, F. Kaess, J. Tweedie, P. Reddy, R. Kirste, Z. Sitar, and R. Collazo, J. Appl. Phys. **127**, 045702 (2020).

[13] K. Alberi and M. A. Scarpulla, J. Appl. Phys. **123**, 185702 (2018).

[14] K. Alberi and M. A. Scarpulla, Sci. Rep. **6**, 27954 (2016).

[15] P. Reddy, M. P. Hoffmann, F. Kaess, Z. Bryan, I. Bryan, M. Bobea, A. Klump, J. Tweedie, R. Kirste, S. Mita, M. Gerhold, R. Collazo, and Z. Sitar, J. Appl. Phys. **120**, 185704 (2016).

[16] Y.-G. Xu, P. Zhang, G.-J. Zhu, J.-H. Yang, and X.-G. Gong, J. Phys. Chem. Lett. **13**, 2474 (2022).

[17] C. E. Sanders, D. A. Beaton, R. C. Reedy, and K. Alberi, Appl. Phys. Lett. **106**, 182105 (2015).

[18] S.-H. Wei and S. B. Zhang, Phys. Rev. B **66**, 155211 (2002).

[19] C. Freysoldt, B. Grabowski, T. Hickel, J. Neugebauer, G. Kresse, A. Janotti, and C. G. Van de Walle, Rev. Mod. Phys. **86**, 253 (2014).

[20] S. M. Sze, Y. Li, and K. K. Ng, *Physics of Semiconductor Devices* (Wiley, New York, 2021).

[21] S. S. X. Li, *Semiconductor Physical Electronics* (Springer, New York, 2012).

[22] J. G. Simmons and G. W. Taylor, Phys. Rev. B **4**, 502 (1971).

[23] K. Kumakura, T. Makimoto, N. Kobayashi, T. Hashizume, T. Fukui, and H. Hasegawa, Appl. Phys. Lett. **86**, 052105 (2005).

[24] C. Stampfl and C. G. Van de Walle, Appl. Phys. Lett. **72**, 459 (1998).

[25] C. G. Van de Walle and J. Neugebauer, J. Appl. Phys. **95**, 3851 (2004).

[26] G. Miceli and A. Pasquarello, Phys. Rev. B **93**, 165207 (2016).

[27] J. Buckeridge, C. R. A. Catlow, D. O. Scanlon, T. W. Keal, P. Sherwood, M. Miskufova, A. Walsh, S. M. Woodley, and A. A. Sokol, Phys. Rev. Lett. **114**, 016405 (2015).

[28] I. P. Smorchkova, E. Haus, B. Heying, P. Kozodoy, P. Fini, J. P. Ibbetson, S. Keller, S. P. DenBaars, J. S. Speck, and U. K. Mishra, Appl. Phys. Lett. **76**, 718 (2000).

[29] A. Bhattacharyya, W. Li, J. Cabalu, T. D. Moustakas, D. J. Smith, and R. L. Hervig, Appl. Phys. Lett. **85**, 4956 (2004).

[30] A. Feduniewicz, C. Skierbiszewski, M. Siekacz, Z. R. Wasilewski, I. Sproule, S. Grzanka, R. Jakieła, J. Borysiuk, G. Kamler, E. Litwin-Staszewska, R. Czernecki, M. Boćkowski, and S. Porowski, J. Cryst. Growth **278**, 443 (2005).

[31] J. Heyd, G. E. Scuseria, and M. Ernzerhof, J. Chem. Phys. **118**, 8207 (2003).

[32] G. Kresse and J. Furthmüller, Phys. Rev. B **54**, 11169 (1996).

[33] Q. Yan, A. Janotti, M. Scheffler, and C. G. Van de Walle, Appl. Phys. Lett. **100**, 142110 (2012).

[34] J. L. Lyons and C. G. Van de Walle, npj Comput. Mater. **3**, 12 (2017).

[35] X. Cai, J. Yang, P. Zhang, and S.-H. Wei, Phys. Rev. Appl. **11**, 034019 (2019).

[36] Y. Zhong, K. S. Wong, W. Zhang, and D. C. Look, Appl. Phys. Lett. **89**, 022108 (2006).

[37] U. Kaufmann, P. Schlotter, H. Obloh, K. Köhler, and M. Maier, Phys. Rev. B **62**, 10867 (2000).

[38] M. E. Levinshtein, S. L. Rumyantsev, and M. S. Shur, *Properties of Advanced Semiconductor Materials: GaN, AIN, InN, BN, SiC, SiGe* (Wiley, New York, 2001).

[39] M. Brendel, A. Kruse, H. Jönen, L. Hoffmann, H. Bremers, U. Rossow, and A. Hangleiter, Appl. Phys. Lett. **99**, 031106 (2011).