

Erratum: Charge-state stability of color centers in wide band gap semiconductors [Phys. Rev. B **108**, 235208 (2023)]

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Based on an error that was pointed out to us, the solution to the differential equation in our paper used to determine the timescales for charge transfer between dopants was corrected. All findings related to the timescales obtained from those results were corrected as well.

III. THEORETICAL APPROACH

A. Thermally driven charge transfer

The likelihood that the electron has enough initial kinetic energy to overcome the ionizing potential energy and recover the neutral system is given by a Fermi-Dirac distribution. We consider the donor level E_{F_D} to be associated with an ionized donor-dopant D and the acceptor level E_{F_A} to be associated with an ionized color center A. We will argue below that the required initial kinetic energy K_{initial} is equal to the difference between the adiabatic charge-transition levels E_{F_D} and E_{F_A} for defects D and A, respectively, up to a correction of order $k_B T$. We can therefore write the expected rate of charge transfer as

$$\langle \Gamma \rangle \approx \int_{t_0}^{\infty} dt \frac{1}{t - t_0} \frac{|\hbar \mathbf{k}(t) \cdot \Delta \mathbf{r}|}{m^* |\Delta \mathbf{r}|^2} \int_{t_0}^t dt' \frac{\hbar \mathbf{k}(t') \cdot \Delta \mathbf{r}}{m^* |\Delta \mathbf{r}|^2} \times \frac{\delta \left(1 - \frac{\int_{t_0}^t d\tilde{t} \hbar \mathbf{k}(\tilde{t}) \cdot \Delta \mathbf{r}}{m^* |\Delta \mathbf{r}|^2} \right)}{\exp \left[(E_{F_D} - E_{F_A}) / k_B T \right] + 1}, \quad (1)$$

where T is the temperature and k_B is the Boltzmann constant. The deionization probability is modeled through the Fermi-Dirac distribution since we consider thermal processes for the charge recombination and not processes involving optical excitations.

C. Computing the momentum due to electric forces

At every point in time, the charge must have enough energy to sustain motion along the path between the defects. To compute the necessary momentum for an electron moving between the defects, we recognize that the momentum must be sufficient to overcome the ionizing electromagnetic potential energy. We note that when the charge approached defect Y from defect X a built-in field emerged to cancel the ionizing field. To capture the emergence of the built-in field, we employ an energy conservation argument. Effectively, our argument is that the sum of the potential energy leading to the ionization of the defect pair and the kinetic energy of the electron must be conserved, so that $U + K = U(K = 0)$. Thus, one finds

$$U = U(K = 0) - K = e[\phi(\mathbf{r}_X) - \phi(\mathbf{r}_Y)] - \frac{\hbar^2 k^2}{2m^*}. \quad (2)$$

Above, the electromagnetic potential energy at $K = 0$, $U(K = 0)$, reflects the relative formation energies associated with the placement of the electron that traveled from defect X to defect Y. A more general potential would allow for the inclusion of arbitrary external fields. The value of the potential energy landscape is defined in the manner given in Eq. (2) at the location of defect X so that its value at the location of defect Y can be set to zero. We correct the solution to the differential equation in the original paper and additionally generalize the differential equation $\frac{d(\hbar \mathbf{k})}{dt} = -\nabla U \supset -\frac{U}{|\mathbf{r}|} \frac{\mathbf{r}}{|\mathbf{r}|}$ by introducing a real parameter α that is independent of $\mathbf{r}$ and t and that multiplies the right-hand side of the differential equation such that $-\nabla U \supset -\frac{U}{|\mathbf{r}|} \frac{\mathbf{r}}{|\mathbf{r}|} \rightarrow -\nabla U \supset -\alpha \frac{U}{|\mathbf{r}|} \frac{\mathbf{r}}{|\mathbf{r}|}$. This approach leverages conservation of energy so that the canceling of the ionizing field by the built-in field can be modeled. The emergence of a built-in field that cancels the ionizing field, however, is only recovered if $\alpha > 1$.

To explicitly determine the required momentum as a function of time, we apply the second law of motion and, motivated by the small-distance approximation to the gradient with forward differences, we employ the limiting case of $\alpha \rightarrow 1^+$ with the

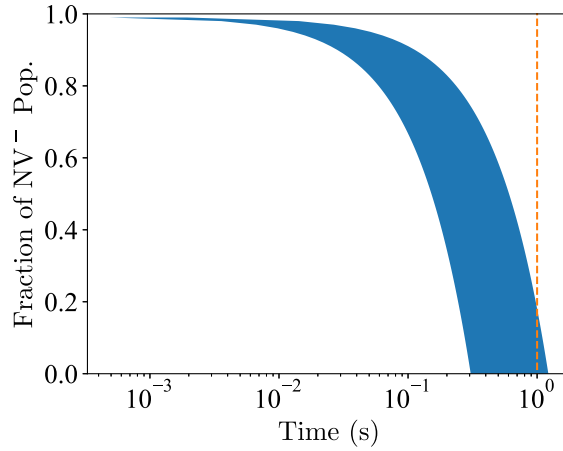


FIG. 1. Fraction of NV^- population remaining as a function of time, calculated via Eqs. (12) and (13) in our paper with $T = 300$ K. We model charge as undergoing transfer from NV^- to N_C^+ . The ionizing dopant concentration is $n_\text{X} = \frac{5 \times 10^8 \text{ cm}^{-2}}{d_\text{max}}$, using an estimated maximum implantation depth of $d_\text{max} = (3.5 \text{ nm keV}^{-1})E_\text{imp}$ where E_imp is the implantation energy [4]. We employ $E_\text{imp} = 3$ keV [2]. The light-blue shaded region represents the result of introducing a shift in E_F_A of $0.03 \text{ eV} \lesssim \Delta E_\text{F}_\text{A} \lesssim 0.07 \text{ eV}$ and of applying the transformation $E_\text{F}_\text{D} \rightarrow (E_\text{F}_\text{D} + 3.4 \text{ eV})/2$. The orange dashed line indicates experimental results for the timescale associated with charge-state decay of four representative individual NV^- centers in sample A with final relative populations between $p = 0.76$ and $p = 0.93$ [2]. Since the four individual NV^- centers were representative, the fraction of the NV^- population remaining after the charge-state decay of each center can lie anywhere between 0 and 1.

origin at the location of defect Y to obtain

$$\frac{d(\hbar \mathbf{k})}{dt} = -\nabla U \supset -\alpha \frac{U}{|\mathbf{r}|} \frac{\mathbf{r}}{|\mathbf{r}|} \Big|_{\alpha \rightarrow 1^+}. \quad (3)$$

In the limit $\alpha \rightarrow 1^+$, it is identically true that at every point $-\nabla U = -\frac{\Delta U}{|\Delta \mathbf{r}|} \frac{\Delta \mathbf{r}}{|\Delta \mathbf{r}|} = -\frac{U}{|\mathbf{r}|} \frac{\mathbf{r}}{|\mathbf{r}|}$, where the difference ΔU is taken by subtracting the potential's value at a given point from its value at the origin with $\alpha \rightarrow 1^+$ and the displacement $\Delta \mathbf{r}$ is taken from the given point to the origin. The nonrelativistic limit is applied above, which is justified by the fact that the maximum speed an electron can attain according to our calculations is less than $0.002c$, where c is the speed of light. Once the electron had arrived at defect Y from defect X, the kinetic energy would be dissipated in a process akin to the Mössbauer effect so that there would be no need to produce a large initial reversal of momentum. Therefore, in our picture where the electron retraces its steps, given an initial (really final) speed corresponding to a kinetic energy $E_\text{thermal} = k_B T$ in a random direction at an angle θ with respect to the radial direction,

$$\frac{dr}{dt} = \lim_{\alpha \rightarrow 1^+} \pm \sqrt{2/m^* \left[U(K=0) - \left(\frac{r}{r_0} \right)^\alpha [U(K=0) - k_B T \cos^2(\theta)] \right]} \quad (4)$$

$$= \pm \sqrt{2/m^* \left[U(K=0) - \left(\frac{r}{r_0} \right) [U(K=0) - k_B T \cos^2(\theta)] \right]}. \quad (5)$$

After writing $\hbar \mathbf{k} = m^* \frac{d\mathbf{r}}{dt}$, the relation $\frac{d^2 r}{dt^2} = \frac{1}{2} \frac{d(\frac{dr}{dt})^2}{dr}$ is used to obtain Eq. (5). We neglect $\frac{d\theta}{dt}$ and $\frac{d^2 \theta}{dt^2}$ since, in our work, $k_B T \ll U(K=0) = e[\phi(\mathbf{r}_\text{X}) - \phi(\mathbf{r}_\text{Y})] = E_\text{F}_\text{D} - E_\text{F}_\text{A}$, where we used the definition of the donor and acceptor levels [1].

In more detail, the barrier at zero temperature (in the absence of phonons) is given by $E_\text{F}_\text{D} - E_\text{F}_\text{A}$. At finite temperature (in the presence of phonons), the barrier is shifted by $-E_\text{initial} = -k_B T \cos^2(\theta) \text{sgn}[\cos(\theta)]$. Averaging this shift over all θ (from $\theta = 0$ to $\theta = \pi$) should give zero for the net shift of the barrier. The barrier is in the argument of an exponential, however, so that the contributions when $\text{sgn}[\cos(\theta)]$ is negative carry more weight in the average than the contributions when $\text{sgn}[\cos(\theta)]$ is positive. Thus, the effective barrier (the barrier we would obtain if we replaced the timescale expression that averages over θ with a timescale expression that employs a single fixed value for the barrier) is higher than the barrier obtained by neglecting the thermal correction. Indeed, at population fractions of approximately 76% and 93% for NV^- centers, the estimates for the charge-state decay time computed without the thermal correction yield values that are, respectively, approximately 1.27 and 1.28 times smaller than the values reported in Fig. 1. Therefore, the room temperature (300 K) contribution of phonons is to increase the barrier by approximately $k_B T \ln(1.27) \approx 0.00618 \text{ eV}$ and $k_B T \ln(1.28) \approx 0.00638 \text{ eV}$, respectively.

Care must be applied if $\theta > \pi/2$ in which case we must first integrate with positive velocity from $r = r_0$ to $r = r_0 \left(\frac{U(K=0)}{[U(K=0) - k_B T \cos^2(\theta)]} \right)$ and then back from $r = r_0 \left(\frac{U(K=0)}{[U(K=0) - k_B T \cos^2(\theta)]} \right)$ to $r = r_0$ with negative velocity before performing the integral between $r = r_0$ and $r = 0$ with negative velocity.

IV. RESULTS AND DISCUSSION

B. Effect of defect species and concentration on charge-conversion timescales

To determine timescales for charge transfer between ionized defect species, we apply Eqs. (12) and (13) in our paper for an ionized color center with acceptor level E_{F_A} transferring an electron to an ionized donor dopant with donor level E_{F_D} . The acceptor and donor levels serving as E_{F_A} and E_{F_D} , measured relative to the valence band maximum, are given by $\epsilon^{\text{NV}}(0/-) \approx 2.8$ eV and $\epsilon^{\text{Nc}}(0/+) \approx 3.6$ eV, respectively. An effective mass of $m^* \approx 1.48m_e$ is obtained from fitting the band structure in Ref. [1]. We account for the fact that the charge-state decay of individual NV^- centers measured in the Yuan *et al.* experiment was to a steady-state relative population greater than 0.5 [2], where 0.5 is the value corresponding to local pinning of the Fermi level at $\epsilon^{\text{NV}}(0/-)$, by introducing a shift in E_{F_A} such that the local Fermi level E_{F_A} would produce a relative NV^- population that would correspond to the experimentally measured value. Explicitly, for a final relative population of p , the shift is $\Delta E_{F_A} = k_B T \ln \left(\frac{(1-p_0)p}{p_0(1-p)} \right)$, where $p_0 = 0.5$. This result is obtained by considering the relative populations of the charge states of a single NV defect. Since we are considering the relative populations for a single defect, we can drop the contribution from configurational entropy. Therefore, the relative population of the NV^- state is given by

$$p = \frac{\exp \left\{ -[\Delta H_f(\text{NV}^-, \{\mu_i^{\text{NV}}\}, 0) - E_F]/k_B T \right\}}{\exp \left[-\{\Delta H_f(\text{NV}^-, \{\mu_i^{\text{NV}}\}, 0) - E_F\}/k_B T \right] + \exp \left[-\Delta H_f(\text{NV}^0, \{\mu_i^{\text{NV}}\}, 0)/k_B T \right]}, \quad (6)$$

where we have assumed that the relative populations of the charge states other than 0 and -1 are negligible since the Fermi level is pinned near the $\epsilon^{\text{NV}}(0/-)$ charge-transition level and used the relation $\Delta H_f(\text{NV}^-, \{\mu_i^{\text{NV}}\}, E_F) = \Delta H_f(\text{NV}^-, \{\mu_i^{\text{NV}}\}, 0) - E_F$ [1]. If we define

$$p_0 = \frac{\exp \left\{ -[\Delta H_f(\text{NV}^-, \{\mu_i^{\text{NV}}\}, 0) - \epsilon^{\text{NV}}(0/-)]/k_B T \right\}}{\exp \left[-\{\Delta H_f(\text{NV}^-, \{\mu_i^{\text{NV}}\}, 0) - \epsilon^{\text{NV}}(0/-)\}/k_B T \right] + \exp \left[-\Delta H_f(\text{NV}^0, \{\mu_i^{\text{NV}}\}, 0)/k_B T \right]}, \quad (7)$$

and write $E_F = \Delta E_F + \epsilon^{\text{NV}}(0/-)$, then it follows immediately that

$$\Delta E_F = k_B T \ln \left(\frac{(1-p_0)p}{p_0(1-p)} \right). \quad (8)$$

The maximum shift is $\Delta E_{F_A} \approx 0.07$ eV and the minimum shift is $\Delta E_{F_A} \approx 0.03$ eV. The corresponding values of p are 0.93 and 0.76, respectively [2]. We also account for the effect of the surface, which we assume to have an etherlike termination [3], so that a donor level measured relative to the valence band maximum of 3.4 eV [3,4] is induced. For NV^- centers near the surface the number of ionized surface donors should be commensurate with the number of ionized bulk donors [4], so we can employ an effective E_{F_D} given by averaging the donor-level values [$E_{F_D} \rightarrow (E_{F_D} + 3.4 \text{ eV})/2$]. Such averaging would also bring our earlier results in better agreement with experimental results at shallow implantation depths [1,4]. The result of these corrections produces good agreement with experiment (see Fig. 1).

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