

Supplementary material: effect of strain on the dark current-voltage characteristic of silicon heterojunction solar cells

L. Guin,^{1,2} P. Roca i Cabarrocas,² M. E. Jabbour,^{1,3} and N. Triantafyllidis^{1,3,4}

¹*LMS, École polytechnique, CNRS, Institut polytechnique de Paris, 91128 Palaiseau, France*

²*LPICM, École polytechnique, CNRS, Institut polytechnique de Paris, 91128 Palaiseau, France*

³*Département de Mécanique, École polytechnique, 91128 Palaiseau, France*

⁴*Aerospace Engineering Department & Mechanical Engineering Department (emeritus), The University of Michigan, Ann Arbor, MI 48109-2140, USA*

In this supplementary material, we present the strain dependence of the electronic parameters of silicon for an arbitrary strain triaxiality. To this end, we use the results from the solid state physics literature on the dependence on strain of the properties of the subbands of the conduction and valence bands of silicon to derive an equivalent two-band formulation for the effective strain dependence of the band edges and densities of states. In sum, we derive the following quantities:

$$\begin{cases} \Delta E_c(\boldsymbol{\varepsilon}) = E_c(\boldsymbol{\varepsilon}) - E_c^r, & \Delta E_v(\boldsymbol{\varepsilon}) = E_v(\boldsymbol{\varepsilon}) - E_v^r, \\ \Delta N_c(\boldsymbol{\varepsilon}) = N_c(\boldsymbol{\varepsilon}) - N_c^r, & \Delta N_v(\boldsymbol{\varepsilon}) = N_v(\boldsymbol{\varepsilon}) - N_v^r, \end{cases} \quad (\text{S1})$$

as well as the changes in the rank-2 tensorial mobilities,

$$\Delta \mathbf{M}_n(\boldsymbol{\varepsilon}) = \mathbf{M}_n(\boldsymbol{\varepsilon}) - \mathbf{M}_n^r, \quad \Delta \mathbf{M}_p(\boldsymbol{\varepsilon}) = \mathbf{M}_p(\boldsymbol{\varepsilon}) - \mathbf{M}_p^r, \quad (\text{S2})$$

where the superscript r denotes the relaxed state of the crystal ($\boldsymbol{\varepsilon} = \mathbf{0}$).

I. REDUCTION OF THE BAND STRUCTURE TO A TWO BANDS DESCRIPTION

The energy band structure of silicon has six subbands in the conduction band and two subbands—called heavy hole band and light hole band—in the valence band (a third subband of the valence band, called spin-orbit band, can be neglected as justified subsequently). Band structure computations performed on the strained crystal allows to quantify the strain-induced changes in each subband. In this section, we shall reduce the multiple band picture of solid state physics to a simplified description with one effective conduction band and one effective valence band, with strain-induced changes equivalent to the compiled effects on the subbands.

A. Conduction band

First, consider the conduction band of silicon. Its six subbands have, in the relaxed state, equal Density Of States (DOS), denoted by $N_{sc,r}$ (the index sc indicates a Subband of the Conduction band and r the Relaxed state $\boldsymbol{\varepsilon} = \mathbf{0}$), and equal edge energy corresponding to the edge energy of the effective conduction band $E_{c,r}$. Under an applied small strain $\boldsymbol{\varepsilon}$, the edge energy of the m conduction subband changes by the quantity $\Delta E_{sc}^m(\boldsymbol{\varepsilon})$, while the change in effective density of states is much smaller and can be neglected.^{S1} The computation of the change in band edge $\Delta E_{sc}^m(\boldsymbol{\varepsilon})$ is treated with the deformation potential theory that was introduced by Bardeen and Shockley^{S2} and further developed in Refs. S3 and S4. It is usually modeled with the *dilational deformation potential* Ξ_d and *shear deformation potential* Ξ_u by:

$$\Delta E_{sc}^m(\boldsymbol{\varepsilon}) = (\Xi_d \mathbf{I} + \Xi_u \mathbf{k}^m \otimes \mathbf{k}^m) : \boldsymbol{\varepsilon}, \quad (\text{S3})$$

where \mathbf{k}^m is the unit vector associated to the direction of the band m in the \mathbf{k} -space (reciprocal to the physical space).

Let $\mathcal{B}_M = (\mathbf{e}_1, \mathbf{e}_2, \mathbf{e}_3)$, the basis aligned with the principal crystallographic directions $\langle 100 \rangle$ of silicon (index M of \mathcal{B}_M is for material, as it is attached to the directions of the material), the \mathbf{k}^m vectors are $\pm \mathbf{e}_1, \pm \mathbf{e}_2, \pm \mathbf{e}_3$ for the subbands $m = 1, 4, m = 2, 5$, and $m = 3, 6$, respectively. Values for Ξ_d and Ξ_u vary in the literature by about 10 %. We take the values from Ref. S3: $\Xi_d = 1.1$ eV and $\Xi_u = 10.5$ eV.

We now introduce a unique effective conduction band with DOS N_c and edge energy $E_c(\boldsymbol{\varepsilon})$. These properties—and their strain dependence—are determined by the equality, at first order in strain, of the expressions of density of electron in the effective band description and in the multiple-band model.

In the multiple-band description, the density of electrons $n(\varepsilon)$ is given by^{S5}

$$n(\varepsilon) = \sum_{m=1}^6 N_{sc} \exp \left[- (E_c^r + \Delta E_{sc}^m(\varepsilon) - E_{F_n}(\varepsilon)) / k_B T \right], \quad (\text{S4})$$

where $E_{F_n}(\varepsilon)$ is the quasi-Fermi level for electrons. Likewise, in the one-band description, the density of electrons reads

$$n(\varepsilon) = N_c \exp \left[- (E_c^r + \Delta E_c(\varepsilon) - E_{F_n}(\varepsilon)) / k_B T \right]. \quad (\text{S5})$$

By letting,

$$N_c = 6N_{sc}, \quad \Delta E_c(\varepsilon) = -k_B T \ln \left(\frac{1}{6} \sum_{m=1}^6 \exp \left[- \Delta E_{sc}^m(\varepsilon) / k_B T \right] \right), \quad (\text{S6})$$

the equality of electron densities in the two descriptions Eq. (S4) and Eq. (S5) is satisfied. With the aim of developing a first order linear theory of the effect of strain on semiconductors, we linearize Eq. (S6) for small strain-induced changes:

$$\Delta E_c(\varepsilon) = \frac{1}{6} \sum_{m=1}^6 \Delta E_{sc}^m(\varepsilon). \quad (\text{S7})$$

Finally, inserting Eq. (S3) in Eq. (S7) yields

$$\Delta E_c(\varepsilon) = \left(\Xi_d + \frac{1}{3} \Xi_u \right) \mathbf{I} : \varepsilon. \quad (\text{S8})$$

B. Valence band

Second, consider the valence band comprised of the heavy hole band and light hole band. While these two bands have the same energy level in the relaxed state, there also exists a third subband, the spin-orbit coupling band, lying at a lower energy level than the two others. As such, this subband contributes much less to the density of holes and can be neglected. In the same way as for the conduction band, we derive an equivalent one-band description with the additional difficulty that the densities of states of the heavy and light hole bands depend significantly on strain.

Denote by $\Delta E_{sv}^l(\varepsilon)$ and $\Delta E_{sv}^h(\varepsilon)$ the changes in band edge energy of the light and heavy hole subbands with respect to their common level in the relaxed state E_v^r and let $\Delta N_{sv}^l(\varepsilon)$ and $\Delta N_{sv}^h(\varepsilon)$ the changes in DOS of these two subbands. In the multiple-band description, the density of holes $p(\varepsilon)$ is given by

$$p(\varepsilon) = \left(\left(N_{sv,r}^l + \Delta N_{sv}^l(\varepsilon) \right) \exp \left[\Delta E_{sv}^l(\varepsilon) / k_B T \right] + \left(N_{sv,r}^h + \Delta N_{sv}^h(\varepsilon) \right) \exp \left[\Delta E_{sv}^h(\varepsilon) / k_B T \right] \right) \times \exp \left[(E_v^r - E_{F_p}(\varepsilon)) / k_B T \right], \quad (\text{S9})$$

where $E_{F_p}(\varepsilon)$ is the quasi-Fermi level of holes.

In the one-band description of the valence band, the density of holes reads

$$p(\varepsilon) = \left(N_v^r + \Delta N_v(\varepsilon) \right) \exp \left[(E_v^r + \Delta E_v(\varepsilon) - E_{F_p}(\varepsilon)) / k_B T \right], \quad (\text{S10})$$

where $\Delta N_v(\varepsilon)$ and $\Delta E_v(\varepsilon)$ are the effective change of the one-band density of states and energy level to be computed from the knowledge on the subbands. Equality of Eq. (S9) and Eq. (S10) yields, at first order in ε ,

$$\begin{aligned} \Delta N_v(\varepsilon) &= \Delta N_{sv}^l(\varepsilon) + \Delta N_{sv}^h(\varepsilon), \\ \Delta E_v(\varepsilon) &= \frac{N_{sv,r}^l}{N_v^r} \Delta E_{sv}^l(\varepsilon) + \frac{N_{sv,r}^h}{N_v^r} \Delta E_{sv}^h(\varepsilon). \end{aligned} \quad (\text{S11})$$

In sum, the strain dependence of the equivalent one-band quantities has been expressed as function of the strain dependence of the subband quantities. The latter can be found in the solid state physics literature, in particular the change in subband energy level is given by Kanda^{S6}, for $u = h, l$,

$$\Delta E_{sv}^u(\varepsilon) = a \mathbf{I} : \varepsilon \pm \left(\frac{b^2}{2} \left((\varepsilon_{11} - \varepsilon_{22})^2 + (\varepsilon_{11} - \varepsilon_{33})^2 + (\varepsilon_{33} - \varepsilon_{22})^2 \right) + d^2 (\varepsilon_{12}^2 + \varepsilon_{13}^2 + \varepsilon_{23}^2) \right)^{1/2}, \quad (\text{S12})$$

where the plus sign is for the heavy hole band and the minus sign for the light hole band^{S1} and a, b and d are the valence band deformation potentials for which we retain the most recent values from Ref. S7: $a = 2.1 \text{ eV}$, $b = -2.33 \text{ eV}$ and $d = -4.75 \text{ eV}$. For the effective description of the valence band, $\Delta E_v(\varepsilon)$ is obtained combining Eq. (S11) and Eq. (S12) with $N_{sv,r}^h/N_v^r = 0.84$ and $N_{sv,r}^l/N_v^r = 0.16$.^{S8}

While it has been recognized early that, unlike the conduction band, the effective density of states of the valence band depends on strain^{S4,S6,S9} it is only recently that Creemer^{S1} pointed out that the change in DOS of the valence band contributes significantly to the piezojunction effect, in particular at relatively moderate strains (a few tenth of percent). We do not have an analytical expression valid for an arbitrary triaxial strain state of that strain dependence and therefore assume an hydrostatic relation, which we calibrate from the band calculations under uniaxial strain of Ref. S1. In addition, these band calculations reflect a symmetric behavior between tensile and compressive strains, which we account for. The hydrostatic strain dependence is a strong assumption and we should, in the following, keep in mind that the estimated contribution to the change in electric current induced by the modification of the valence band density of states is very uncertain. In sum, we write, for each valence subband $u = h, l$,

$$\Delta N_{sv}^u(\varepsilon) = \tilde{N}_{sv}^u |\mathbf{I} : \varepsilon|, \quad (\text{S13})$$

where the scalar coefficients $\tilde{N}_{sv}^l = 240N_{sv,r}^l$ and $\tilde{N}_{sv}^h = -240N_{sv,r}^h$ are computed from Figure 2.16 of Ref. S1. Combining Eq. (S11) with Eq. (S13), we obtain the strain dependence of the effective valence band density of states:

$$\Delta N_v(\varepsilon) = \tilde{N}_v |\mathbf{I} : \varepsilon|, \quad (\text{S14})$$

with $\tilde{N}_v = -170N_v^r$. Relation Eq. (S14) is only an approximate estimation of the strain effect on the DOS of the valence band. A detailed band calculation for general strain is required to derive a more exact strain dependence with full account of strain triaxiality.

II. CHANGE IN MOBILITIES

A. General Theory

The change with strain of the mobility of electrons and holes is equal to the opposite of the change in resistivity. The latter is measured in experiments^{S1,S10} and, as such, yields the mobility changes of electrons and holes in the effective one-band description. Thus, there is no need to resort to the subband description for mobilities. The changes in resistivity are usually expressed with respect to the stress tensor σ with the rank-4 piezoresistive tensors Π_n and Π_p for electrons and holes.^{S1,S10,S11} Using those tensors and the constitutive relation $\sigma = \mathbf{c} : \varepsilon$ with \mathbf{c} the elasticity tensor, the relative change in the ij -coefficient of the mobility tensor can be expressed with the small strain tensor ε

$$\frac{(\Delta \mathbf{M}_q)_{ij}(\varepsilon)}{(\mathbf{M}_q^r)_{ij}} = -(\Pi_q : \mathbf{c} : \varepsilon)_{ij}, \quad (\text{S15})$$

for $q = n, p$ and for every $i, j = 1, 2, 3$, without summation on the repeated indices.

a. Practical calculation of the effect of strain on mobilities Equation. (S15) can be expressed in matrix form using the Voigt notation. Denote by $[\mathbf{a}]^{\mathcal{B}}$ the matrix of the coefficients of a tensor \mathbf{a} of rank-1 or -2 in the basis \mathcal{B} and $\{\mathbf{A}\}^{\mathcal{B}}$ the representation, in Voigt notation, of a properly symmetric tensor \mathbf{A} of rank-2 or -4 in basis \mathcal{B} . For any rank-2 tensor, we have the usual relation between classical and Voigt notations,

$$\begin{aligned} \{\mathbf{A}\}_1 &= [\mathbf{A}]_{11}, & \{\mathbf{A}\}_2 &= [\mathbf{A}]_{22}, & \{\mathbf{A}\}_3 &= [\mathbf{A}]_{33}, \\ \{\mathbf{A}\}_4 &= [\mathbf{A}]_{23}, & \{\mathbf{A}\}_5 &= [\mathbf{A}]_{13}, & \{\mathbf{A}\}_6 &= [\mathbf{A}]_{12}, \end{aligned} \quad (\text{S16})$$

with an exception for the extradiagonal terms of the strain tensor ε ,

$$\{\varepsilon\}_4 = 2[\varepsilon]_{23}, \quad \{\varepsilon\}_5 = 2[\varepsilon]_{13}, \quad \{\varepsilon\}_6 = 2[\varepsilon]_{12}. \quad (\text{S17})$$

This allows us to rewrite Eq. (S15) as

$$\frac{\{\Delta \mathbf{M}_q\}_i(\varepsilon)}{\{\mathbf{M}_q^r\}_i} = -(\{\Pi\}_q \cdot \{\mathbf{c}\} \cdot \{\varepsilon\})_i, \quad (\text{S18})$$

Π_{11}^n	Π_{12}^n	Π_{44}^n	Π_{11}^p	Π_{12}^p	Π_{44}^p
-102.2	53.4	-13.6	6.6	-1.1	138.1

TABLE I. Piezoresistive coefficients in 10^{-11} Pa^{-1} from Ref. S10. For comparison with values obtained by other works see Ref. S1, Table 2.4.

for every $i = 1..6$, where for two rank-2 or -4 tensors \mathbf{A} and \mathbf{B} , $\{\mathbf{A}\} \cdot \{\mathbf{B}\}$ denotes the traditional matrix-matrix or matrix-vector product.

In Voigt notations, due to the cubic symmetries of silicon, in the basis \mathcal{B}_M , the matrices $\{\Pi_q\}$ for $q = n, p$ read^{S10-S12}

$$\{\Pi_q\}^{\mathcal{B}_M} = \begin{pmatrix} \Pi_{11}^q & \Pi_{12}^q & \Pi_{12}^q & 0 & 0 & 0 \\ \Pi_{12}^q & \Pi_{11}^q & \Pi_{12}^q & 0 & 0 & 0 \\ \Pi_{12}^q & \Pi_{12}^q & \Pi_{11}^q & 0 & 0 & 0 \\ 0 & 0 & 0 & \Pi_{44}^q & 0 & 0 \\ 0 & 0 & 0 & 0 & \Pi_{44}^q & 0 \\ 0 & 0 & 0 & 0 & 0 & \Pi_{44}^q \end{pmatrix}, \quad (\text{S19})$$

with the coefficients summarized in Table I. Note the variations up to two orders of magnitude between the different coefficients of Table I, which indicate that the carrier mobilities might be significantly or little affected by the stress depending on both:

1. The stress state (i.e., its triaxiality),
2. The components of the mobility tensor relevant for a particular experiments and which are determined by the directions of electron (resp. hole) current and gradient of electron (resp. hole) electrochemical potential.^{S13}

We also recall that the elasticity tensor \mathbf{c} of silicon in Voigt notation has the same form as Eq. (S19) with coefficients in the basis \mathcal{B}_M , $c_{11} = 166 \text{ GPa}$, $c_{12} = 64 \text{ GPa}$ and $c_{44} = 80 \text{ GPa}$.^{S14}

B. Application to the experiment shown in Fig. 2 of the main article

In the following, we show why the strain dependence in the hole mobility can be neglected for the particular crystallographic directions of the experiment reported in Fig. 2 of the main article. With the basis \mathcal{B}_G of Fig. 2, the component of the mobility tensor involved in hole transport is $M_{p,zz}$. The change with strain of that component is computed using Eq. (S18), which yields by taking the component ε_{yy} for the amplitude of strain (ε_{xx} and ε_{zz} are implicitly accounted for by writing them as a function of ε_{yy}):

$$\frac{\Delta M_{p,zz}}{M_{p,zz}} = -\frac{4c_{11}^2 c_{44} + 4c_{11} c_{12} c_{44} - 8c_{12}^2 c_{44}}{c_{11}^2 + c_{11} c_{12} + 2c_{11} c_{44} - 2c_{12}^2} \Pi_{12}^p \varepsilon_{yy}, \quad (\text{S20})$$

Numerically, for $\varepsilon_{yy} = 1 \times 10^{-3}$ (upper bound in the experiments), the relative change in mobility is only of 0.2% which is very small compared to the changes due to the other phenomena (of the order of 10%). As a result, for the experiment under consideration the influence of mobility can be neglected as mentioned in the main article.

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[S8]These ratio of density of states are obtained as follows: The effective density of states of each subband is related to the effective mass of each subband m^l and m^h by^{S15}

$$N_{sv,r}^u \propto (m^u)^{3/2}, \quad (\text{S21})$$

for $u = l, h$ where $m^l = 0.16m_0$ and $m^h = 0.49m_0$ with m_0 the free-electron mass. In addition, the density of states of the effective valence band is simply,

$$N_v^r = N_{sv,r}^l + N_{sv,r}^h, \quad (\text{S22})$$

which combined with Eq. (S21) yields the ratios of DOS.

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