Giant Poole-Frenkel effect for the shallow dislocation-related hole traps in silicon

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Abstract. The results of a theoretical calculation of the Pool-Frenkel effect due to the strain field of screw and 60º dislocations upon the valence band in silicon, and of a detailed DLTS study of the electrical field impact on carrier emission from the dislocation-related states of two types of bonded samples are presented and discussed. A good agreement between the theory and experiment was established. It is concluded that the large Pool-Frenkel coefficient value that significantly exceeds the value for a Coulomb-like potential is a new distinguishing feature of the hole thermo-emission from dislocation-related levels in silicon.

1. Introduction

During the last few decades, dislocation-related electronic states in the band gap of silicon were intensively studied by means of deep level transient spectroscopy (DLTS) and numerous data were collected (for review see [1]). The main well-known features of the dislocation-related DLTS-signal are the broadening of the DLTS peaks and the logarithmic dependence of their magnitude on the refilling pulse duration. Very recently it was reported [2] that the main hole traps in p-type silicon with a dislocation network (DN) exhibited a strong field-enhanced thermal emission. A linear dependence of the activation energies for the hole emission on the square root of the electric field (the Pool-Frenkel effect) was established. In addition, the Pool-Frenkel coefficient value was found to be different in samples with different dislocation structures, and to exceed the theoretical value for the Coulomb potential. That led to the assumption [2] of a dislocation-strain-related origin of the phenomenon observed.

In this work we performed theoretical calculations of the Pool-Frenkel effect due to the strain field of screw and 60º dislocations for the valence band in silicon, and more detailed experimental investigations of the impact of the electrical field on the carrier emission from the dislocation-related states of similar types of samples produced by silicon direct wafer bonding by means of diverse techniques of capacitance-transient analysis and of transmission electron microscopy (TEM). A good agreement between the theory and experiment was established. From this fact we conclude that giant Pool-Frenkel coefficient value is a new distinguishing feature of 60º dislocations in silicon.
2. Theory of Pool-Frenkel effect due to elastic strains of dislocations

2.1. Isolated dislocations

The Pool-Frenkel effect is a lowering of the potential barrier for carrier thermoemission from a deep level as the result of the composition of its attractive, Coulomb-like potential that is inversely proportional to the distance, \( r \), and of the potential of a uniform electrical field, \( F \) (see figure 1).

The resulting potential is three dimensional (3D) and depends on the angle \( \theta \) between \( F \) and \( r \) as:

\[
V(r) = -q\left(\frac{A}{r} + Fr\cos\theta\right)
\]

It exhibits a maximum at the distance (see figure 1):

\[
r_m = \sqrt{\frac{A}{F\cos\theta}} = \frac{\beta}{2\sqrt{F}},
\]

giving rise to the reduction of the emission activation energy by

\[
\delta E_r = -q\beta\sqrt{F}
\]

where

\[
\beta = 2\sqrt{A\cos\theta}
\]

is the Pool-Frenkel constant and \( q \) is the elemental charge.

For a Coulomb potential \( A=q/4\pi\epsilon \) that gives the maximum \( \beta \)-value of \( 2.22\times10^{-4}\text{V}^{-1/2}\text{cm}^{1/2} \) for \( \cos(\theta)=1 \) corresponding to the one-dimensional (1D) case. The calculation of the field-enhanced emission in the 3D-case needs the integration over spatial angles [3] that can be performed analytically and gives rise to a lower \( \beta \)-value of about \( 2\times10^{-4}\text{V}^{-1/2}\text{cm}^{1/2} \).

The deformation potential of dislocations is also inversely proportional to the distance [4]. Thus, a qualitatively similar field effect on the thermal emission of the carriers from electronic states located close to the dislocation cores can be expected. In the following we perform calculations of the Pool-Frenkel effect for the hole emission from the dislocation-related level to the valance band (\( \Gamma \)-point) in silicon. For this zone point, the theory [5] predicts that both uniaxial and shear components of dislocation deformation tensor can contribute to the deformation potential.

The components of the deformation tensor are usually expressed in the dislocation coordinate system where \( x \) coincides with the dislocation line which is [110] for both screw and 60° dislocations.
in silicon. Two other coordinates directions are arbitrary and we will take \( z \) to be along \([001]\) and \( y \) to be along \([1-10]\) directions.

In this coordinate system, the deformation tensor for screw dislocations consists of two non-diagonal components \( \varepsilon_{xy}, \varepsilon_{zx} \):

\[
\varepsilon_{xy} = -\frac{B_y}{4\pi r}\sin\theta \\
\varepsilon_{zx} = \frac{B_z}{4\pi r}\cos\theta
\]

(5)

For edge dislocations, the tensor consists of three components that also contain hydrostatic deformation \( \varepsilon \):

\[
\varepsilon_{xy} = -\frac{B_y}{4\pi r(1-\nu)}\left(\cos\theta\left\{(1-2\nu)+2\sin^2\theta\right\} + \frac{B_z}{4\pi r(1-\nu)}\left(\sin\theta\left\{(1-2\nu)-2\cos^2\theta\right\}\right)
\]

(6)

\[
\varepsilon_{zx} = \frac{B_z}{4\pi r(1-\nu)}\left(\sin\theta\left\{1-2\cos^2\theta\right\}\right) - \frac{B_y}{4\pi r(1-\nu)}\left(\cos\theta\left\{1-2\sin^2\theta\right\}\right)
\]

\[
\varepsilon = Sp(\varepsilon_n) = \frac{(1-2\nu)}{2\pi r(1-\nu)}\left(B_z\sin\theta-B_y\cos\theta\right)
\]

where \( B_x, B_y \) and \( B_z \) are the projections of the Burgers vectors along corresponding directions, \( r \) is the distance from dislocation, the angle \( \theta \) is counting out from \( z \) axis and \( \nu \) is the Poisson ratio (\( \nu=0.3 \) for Si).

The calculations of the dislocation deformation potential have to be performed in the natural crystal coordinate system that for cubic lattices is \( x'=\[100]\), \( y'=\[010]\), \( z'=\[001]\) [5]. In this system the deformation tensor for the dislocation with an arbitrary Burgers vector can obtained by a 45° rotation of the dislocation coordinates around the \( z \)-axis and has the general form as follows:

\[
\begin{pmatrix}
\frac{\varepsilon_{yy}}{2}+\frac{\varepsilon_{xy}}{2} & \frac{\sqrt{2}}{2}(\varepsilon_{xy}+\varepsilon_{zx}) \\
\frac{\varepsilon_{xy}}{2} & \frac{\varepsilon_{yy}}{2}-\varepsilon_{xy} & \frac{\sqrt{2}}{2}(\varepsilon_{xy}-\varepsilon_{zx}) \\
\frac{\sqrt{2}}{2}(\varepsilon_{zy}+\varepsilon_{zx}) & \frac{\sqrt{2}}{2}(\varepsilon_{zy}-\varepsilon_{zx}) & \frac{\varepsilon_{zz}}{2}
\end{pmatrix}
\]

(7)

Following the deformation potential theory [5] the valence band in silicon at the \( \Gamma \)-point exhibits a shift due to the hydrostatic component, and a splitting into two sub-bands due to shear components of deformation tensor. Taking into account the explicit form of deformation tensor (7), the resulting deformation potential of the dislocation can be written as:

\[
V_{1,2} = aSp(\varepsilon_n) \pm 
\]

\[
\pm \left\{ \frac{b^2}{2}\left[(2\varepsilon_{xy})^2 + (\varepsilon_{zy} - \frac{\varepsilon_{yy}}{2} + \varepsilon_{xy})^2 + (\varepsilon_{zz} - \frac{\varepsilon_{yy}}{2} - \varepsilon_{xy})^2\right] + \frac{d^2}{2}\left[(\varepsilon_{yy} + \varepsilon_{xy})^2 + (\varepsilon_{zy} - \varepsilon_{zx})^2 + \frac{\varepsilon_{zz}^2}{2}\right]\right\}^{1/2}
\]

(8)

where numerical values of the deformation potential constants for the valence band in silicon are \( a=5.1\text{eV}, b=2.2\text{eV} \) and \( d=5.1\text{eV} \).
Using equation (8) together with the explicit form of the deformation components (5) and (6), we calculated the parameters $A=Vr/qB$ and $\beta$ that quantify the Pool-Frenkel effect. In the calculations the electrical field was directed along $z$. For a pure screw dislocations we took $B_z = B = 0.384$ nm. For the $60^\circ$ dislocation, $B_x = B/2$, $B_z = 0.707B$, whereas $B_y$ was either $+B/2$ or $-B/2$ corresponding to those two possible orientations of the $60^\circ$ dislocation with respect to the (001) plane marked as b1 and b2 in figure 2A, respectively.

Figure 2. (A) Orientations of $60^\circ$ (b1, b2) and screw (b3) dislocations in the projection on (110) plane. Dashed line shows the projection of the (001) plane with the dislocation network. Electric field F is directed to [001]. (B) shows the theoretical angle dependence of deformation potential (A-factor) for $60^\circ$ dislocations with the orientations b1 and b2 shown in figure 1A. The angle is counted from the direction [001] that coincides with the direction of electric field.

Figure 2B represents the angle dependences of A-factor for $60^\circ$ dislocations with two possible orientations in the DN plane depicted in figure 2A. The main features of the dependences are: 1) significant splitting of the valence band around the dislocations caused by shear deformations; 2) the lower sub-band forms an attractive potential for most directions that can cause a Pool-Frenkel effect; 3) the shapes of the corresponding potential for the two dislocation orientations are close to each other but shifted by the angle of about $70^\circ$.

Figure 3A shows $\beta(\theta)$ calculated for the lower valence band $V_2$ at the screw, at both types of $60^\circ$ dislocations as well as for a 3D Coulomb potential. One can note that the $\beta(\theta)$ for screw dislocation is rather similar to the one for the Coulomb potential, while for $60^\circ$ dislocations it has a larger maximum value especially for the b1 orientation.

The calculation of the field enhanced emission rate for dislocations was performed making use the integration according to:

$$
\frac{e_p(F)}{e_{p0}} = \frac{1}{2\pi} \left[ \alpha \int_{-\pi/2}^{\pi/2} d\theta \exp\left(\frac{-\delta E_c(\theta)}{kT}\right) + 1 - \alpha \right]
$$

where $\alpha$ is the ratio of the angles where enhanced emission takes place ($\alpha$ is 0.5 for screw and $60^\circ$ dislocation b1, but is 0.325 for $60^\circ$ dislocation b2).

The results of numerical integration of equation (9) for all dislocations as well as the previously reported [3] expression for the 3D Coulomb are presented in figure 3B. At sufficiently high electric fields, all of the curves can be well fitted with the Pool-Frenkel law: $e_p(F)/e_{p0} = \exp(\beta_{\text{eff}}\sqrt{F})$. The curves for the Coulomb potential and for the screw dislocation deformation potential for the valence band coincide practically with each other giving $\beta_{\text{eff}}(b1) \approx 2\times10^{-4} V^{1/2} \text{cm}^{1/2}$. The values for $60^\circ$ dislocations are $\beta_{\text{eff}}(b1) \approx 3.2\times10^{-4} V^{1/2} \text{cm}^{1/2}$ and $\beta_{\text{eff}}(b2) \approx 2.4\times10^{-4} V^{1/2} \text{cm}^{1/2}$. 

The results of numerical integration of equation (9) for all dislocations as well as the previously reported [3] expression for the 3D Coulomb are presented in figure 3B. At sufficiently high electric fields, all of the curves can be well fitted with the Pool-Frenkel law: $e_p(F)/e_{p0} = \exp(\beta_{\text{eff}}\sqrt{F})$. The curves for the Coulomb potential and for the screw dislocation deformation potential for the valence band coincide practically with each other giving $\beta_{\text{eff}}(b1) \approx 2\times10^{-4} V^{1/2} \text{cm}^{1/2}$. The values for $60^\circ$ dislocations are $\beta_{\text{eff}}(b1) \approx 3.2\times10^{-4} V^{1/2} \text{cm}^{1/2}$ and $\beta_{\text{eff}}(b2) \approx 2.4\times10^{-4} V^{1/2} \text{cm}^{1/2}$. 

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Figure 3. Angle dependence of Pool-Frenkel coefficient (A) and relative enhancement of the hole thermoemission under applied electric field (B) for 3D Coulomb (blue dashed line) and for deformation potential of screw (green solid line), 60° dislocation with two orientations depicted in figure 2A: b1 -red short-dashed line, b2- black dashed-dotted line).

2.2. Dislocation network
For the samples under investigation, the interaction of the elastic strains between the dislocations in a network must be taken into consideration that generally results in strain field localization.

Detailed examination of the contribution of different components of deformation tensor to the Pool-Frenkel constant for screw dislocations showed that the most important component is $\varepsilon_{xy}$. Using the explicit expression for the elastic strains of a dislocation row given in [4], we plotted the dependence for this component as a function of the reciprocal distance from the plane of dislocation row (figure 4A) and DN (figure 4B) and compared them with that for the isolated dislocation. The results are presented in figure 4C.

Figure 4. (A) Dislocation row and (B) square dislocation network. (C) shows the deformation of isolated dislocation (long dashed), dislocations in a row A (dashed-dot) and in a square network B (solid). For the DN, the z-coordinate goes through the centre of dislocation segments between the nodes.
One can see that the significant difference of the strains $\varepsilon_{xy}$ from $1/r$ law starts at the distances larger than $z_{\text{crit}}$ being of about $D/5$ and $D/2$ for dislocation row and for DN respectively. Obviously, the Pool-Frenkel law can be observed under application of the electric field above the value $F_{\text{min}}$ that corresponds to Pool-Frenkel radius ($r_m$, equation 2) of about $z_{\text{crit}}$.

The latter value allows one to estimate $F_{\text{min}}$ as a function of $D$ by using relation:

$$F_{\text{min}} > \left(\frac{\beta}{2z_{\text{crit}}}\right)^2$$

or estimate $D_{\text{min}}$ for the given electric field ranges:

$$D_{\text{min}} > (2 \div 5)\frac{\beta}{2\sqrt{F}}$$

where the numbers 2 or 5 relate to DN or to the row, respectively. By using these expressions [4], it can be shown that similar estimates are valid for the row of edge type dislocations as well.

3. Samples and experimental technique

Samples were fabricated by direct bonding of 200 mm, p-type Si wafers with (001) surface orientations in a hydrophilic process, i.e. the surfaces of the wafers were covered with native oxide layer before the bonding process [6]. The doping level of the wafers was $\approx 10^{15}$ atoms/cm$^3$ of boron. A detailed description of the bonding procedure can be found elsewhere [6],[7]. After the bonding and a thinning procedure of the top layer, a dislocation network was located at the depth of 160 nm from the sample surface. In order to dissolve the interfacial native oxide layer, samples were annealed at 1200°C in high purity conditions [6]. After the annealing neither secondary ion mass spectrometry nor TEM investigations revealed any variations of oxygen concentration near to the bonding interface. Wafers were bonded with two different twist angles of about 1 and 3 º and are denoted as Gr-1 and Gr-3 respectively. Both samples have the same small tilt angle of about 0.5° that was a result of wafer polishing.

To produce Schottky contacts for DLTS measurements, 100 nm-thick titanium dots with 1.5 mm diameter were evaporated on the oxide free front surface of all samples. Ohmic contacts were prepared by rubbing of InGa on the rear side of the samples. DLTS measurements were performed by means of transient Fourier spectroscopy system DL-8000 (Accent).

4. Experimental results

DLTS spectra of both samples investigated possess similar features: the main, low-temperature peak (labelled as ST1 in Gr-1 and as ST3 in Gr-3) dominates the spectrum and a set of strongly overlapped DLTS peaks appear at temperatures of 100-250K (for details see [2]). It was also found, that the temperature positions of the ST1 and ST3 peaks were shifted toward lower temperatures with the increase of applied reverse bias, i.e. with the increase of the electric field in the depletion region, as shown in figure 5. Note that the sets of DLTS spectra for Gr-1 and Gr-3 samples presented in figures 5A and 5B were measured with the same refilling pulse voltage, $U_p = -1V$.

Detailed analysis of the shape of the ST1 and ST3 DLTS peaks revealed that their shapes differed from expected for point-like defects. The broadening of DLTS peaks can generally affect the precision of the $E_a$ definition and can be caused either by the widening of the electronic spectrum or by spatial or transient variation of the electric field. That is why we performed another type of the experiment to evaluate the Pool-Frenkel coefficient value, that is isothermal relaxation Spectroscopy (ITS).
ITS measurements were performed at constant temperature under the gradually increasing rate window period using the same correlation procedure as DLTS. Since the response of the DLTS correlator is a function of the product of the emission rate, $e_p$, and the correlator period, $\tau$, the dependence of $\tau$ on the electrical field obtained at a specific level of ITS signal (i.e. keeping the product $e_p\tau$ = constant) will be inversely proportional to the dependence on $e_p$. Thus, when the broadening of a DLTS line is caused by a widening of the electronic spectrum, the dependence of $\ln(e_p)$ on the square root of electric field must have the same slope, $\beta$, for all the ITS signal level. Alternatively, when the broadening is caused by electric field variations $\beta$ might vary dependent on the ITS signal level.

Examples of ITS spectra of the Gr-1 and Gr-3 samples measured with different reverse bias voltages, $U_r$, and the same filling pulse voltage $U_p$ = -1V are presented in figure 6. Measurement temperatures were chosen to be 40K for Gr-1 sample and to be 53K for Gr-3 sample that allowed one to use the largest interval $U_r$ voltages for the ITS spectra acquisition inside the usable rate window ranges of our transient recorder.

The electric field at the position of the DN ($d = 160$nm below the front sample surface) for every reverse bias voltage was calculated using the standard relation $F = qN_a(w-d)/\varepsilon$, where $N_a$ is the net acceptor concentration, and $w$ is the SCR-width calculated from capacitance data at the DLTS/ITS measurement temperature. Generally, the charge contained within DN states should be taken into account for the electric field calculations as well. Unfortunately, the ground charge state of the detected traps is not known precisely. Nevertheless, we believe the charge collected at the DN will not significantly modify the results of the field definition since the total charge of the doping impurity inside the space charge region, $eN_a w$, is much larger than the total concentration of all traps detected by DLTS, i.e. $eN_a w > e\Sigma N_{DLTS}$ for all used $U_r$ voltages.
Using the values of the electric field calculated in such a way, dependences of activation enthalpies $E_a$, derived from the DLTS spectra, and $k T \ln(e_p)$ derived from the ITS measurements based upon the square root of electrical field $\sqrt{F}$ were plotted, as shown in figures 7A and 7B, respectively. One can see that all the dependences obtained for both ST1 and ST3 peaks could be well approximated by a straight line, and thus follow the Poole-Frenkel law.

The slopes of the linear dependences obtained, which correspond to Poole-Frenkel coefficients $\beta$, as well as the activation enthalpies, $E_{a0}$ at zero electric field approximated from DLTS data (figure 7A), are summarized in table 1. It should be noted also that $\beta$-values obtained from the ITS-data at different signal levels coincided within the measurement errors, indicating that the broadening of the DLTS spectra arises from the broadened spectra of the electronic states.

**Figure 6.** Sets of ITS spectra of (A) sample Gr-1 and (B) sample Gr-3, measured with different reverse bias voltages. Ordinate axes show the surface trap density, abscissa axes – the natural logarithm of the emission time constant $\tau$. ITS-scan parameters: measurement temperatures are 40K for Gr-1 sample and 53K for Gr-3 sample, filling pulse duration $t_p=100\mu$s, and filling pulse voltage $U_p=-1V$. Reverse bias voltages, $U_r$, are shown in the legends.

Using the values of the electric field calculated in such a way, dependences of activation enthalpies $E_a$ derived from the DLTS spectra, and $k T \ln(e_p)$ derived from the ITS measurements based upon the square root of electrical field $\sqrt{F}$ were plotted, as shown in figures 7A and 7B, respectively. One can see that all the dependences obtained for both ST1 and ST3 peaks could be well approximated by a straight line, and thus follow the Poole-Frenkel law.

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**Figure 7.** Dependences of the activation enthalpies, $E_a$, derived from (A) DLTS, and (B) the $k T$-corrected logarithm of emission rates derived from ITS dependence on the square root of electric field for the ST1 and ST3 peaks in Gr-1 and Gr-3 samples. Symbols show experimentally obtained values, and straight lines linear approximations.
The $\beta$-values are noticeably larger than those expected for a 3D Coulomb potential, especially for sample Gr-1. The values obtained from the DLTS measurements are slightly bigger than those from the ITS-data. The reason of this discrepancy is not known precisely and might be caused by a systematic error in temperature measurements affecting mostly the determination of the activation energies $E_a$ from Arrhenius plots. The difference between the zero-field activation enthalpy, $E_{a0}$, for the ST1 trap level and that for the ST3 level at about 15 meV is close to their definition error.

|                  | Gr-1 sample | Gr-3 sample |
|------------------|-------------|-------------|
|                  | ST1 peak    | ST3 peak    |
| ITS $\beta$, (10^{-4} \text{ cm}^{1/2} \text{V}^{-1/2})$ | 2.8         | 2.1         |
| DLTS $\beta$, (10^{-4} \text{ cm}^{1/2} \text{V}^{-1/2})$ | 3.0         | 2.4         |
| $E_{a0}$, (eV)   | 0.105       | 0.12        |

5. Discussion

Our theoretical calculations presented in section 2 showed that the $\beta$-coefficient value of the dislocation-related Pool-Frenkel effect depends strongly on the type, on the orientation and on the density of dislocations. Figure 8 shows TEM micrographs of the dislocation structure of the DN of both samples investigated.

Detailed analysis of the structure showed that most of the dislocations in sample Gr-1 (figure 8A) seemed to be 60° dislocations, though the exact direction of Burgers vector could not be defined precisely from TEM data. The structure in figure 8A looks like a row of parallel dislocations separated by distances of about 60 nm rather than a square DN.

The electric field values used in the experiment with this sample started from 14 kV/cm. The minimal distance when the theory of isolated dislocation is still valid can be estimated according to equation (10) for that field is of about 40 nm. Thus, the theoretical conditions are satisfied and the predicted Pool-Frenkel coefficient value is expected to be about $3 \times 10^{-4} \text{cm}^{1/2} \text{V}^{-1/2}$ for the case of the most favourable orientation $b_1$ of 60° dislocations in the DN shown in figure 2. This is in good agreement with the $\beta$-value for this sample (see table 1).

Figure 8. Dark field TEM images of the samples under investigation. (A) sample Gr-1 and (B) sample Gr-3.
The dislocation structure of sample Gr-3 consists of square mesh of perfectly straight screw dislocations (only one set of them is visible in figure 8B due to particular diffraction conditions) and the rows of curved 60° dislocations that are inclined to the screw dislocation lines on average at an angle of about 30°. The inter-dislocation distances for screw dislocations are of about 7 nm, while for the 60° dislocations they are varying from 30 to 50 nm. For the electric field ranges used in the experiments (see figure 7) the Pool-Frenkel radius is estimated to be of 8-14 nm for the mesh and 20-33 nm for the row. Hence, the validity of the theory for isolated dislocation is satisfied for 60° dislocations but not for screw dislocations. Thus, the screw dislocations have to be ruled out of the consideration as a possible origin for the observed Pool-Frenkel effect. The Pool-Frenkel coefficient value obtained from experiment $\beta \approx (2.1-2.4) \times 10^{-7} \text{V}^{1/2} \text{cm}^{-1/2}$ corresponds to the theoretically predicted value for 60° dislocation in the orientation $b_2$ in figure 2.

The difference between the experimental $\beta$-value for the Gr-1 and Gr-3 samples can be then explained due to different crystallographic orientations of the handle and the top bonded wafers. The predominant 60° dislocation orientations $b_1$ or $b_2$ in figure 2 could be realized due to an asymmetry of the tilt misorientation between the handle and the top wafers, for example, when the handle wafer has exact (100) orientation and the tilt between the wafers is due to misorientation of the top wafer only or vice versa. Since the tilt between the bonded wafers was not controlled during the bonding process and arose as the result of wafers polishing such an explanation seems to be reasonable. Nevertheless, one can not exclude that the lower $\beta$ in the Gr-3 sample was due to the interaction of 60° dislocations with screw dislocations giving rise to a zigzag configuration of resulting dislocations [8]. Such a configuration, obviously, could have the strain field that differs significantly from that of a straight dislocation.

6. Conclusion
In conclusion we have demonstrated both theoretically and experimentally a new dislocation-related phenomenon that is the Pool-Frenkel effect caused by elastic strains of dislocations in silicon. We showed that Pool-Frenkel coefficient can reach the value that significantly exceeds the value for a Coulomb-like potential of a singly charged point defect. The presence of dislocations with different Burgers vectors and different orientations with respect to the electric field can cause a drastic broadening of DLTS-peaks.

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