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MODELING THE DENSITY-OF-STATES SPECTRUM UNDER STRAIN IN DOPED SILICON p-Si⟨B, Mn⟩

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A deformation (strain) model of the spectrum of the density of localized states Nss(E,X) in p-Si⟨B,Mn⟩ under uniaxial pressure X is presented. It is shown that shifts of trap levels can be described by the deformation energy Ed = κX, a mechanical analog of kT. At a fixed temperature $T = 77$ K, increasing X leads to a shift and restructuring of the spectrum: thermodonor (TD) levels move toward the conduction band, whereas manganese (Mn) levels shift toward the valence band, which agrees with the opposite trends observed in ρ(X) and μ(X).

Keywords: *Doped silicon; Deformation energy; Uniaxial pressure; Strain-stimulated effects; Density of states; Energy spectrum of Si⟨B,Mn⟩; Si⟨B,TD⟩*
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INTRODUCTION

The influence of mechanical strain on the electronic properties of silicon remains one of the fundamental topics in solid-state physics. A number of studies have established that uniaxial pressure causes a reconstruction of the band structure, changes in charge-carrier mobility, and redistribution of the density of states within the band gap [1–3].

In [1] it was shown that compression along the [1] axis leads to the breakup of oxygen thermodonors (TD), a hysteresis in the resistivity dependence *ρ(X)*, and opposite changes in the mobility *μ(X)* for p-Si⟨B,TD⟩ and p-Si⟨B,Mn⟩. Pressure acts as a physical parameter analogous to temperature, but it operates through the deformation energy *Ed = kX*. In thermodonor samples (TD) it promotes carrier delocalization and a decrease in ρ, whereas in Mn-doped systems it enhances localization and increases the resistance.

It is known that manganese-doped silicon exhibits complex defect structures associated with the formation of magnetic nanoclusters. Experimental studies using electron spin resonance (ESR) have shown that manganese atoms in silicon can form clusters consisting of several atoms located near boron impurities, which significantly affect the electronic and magnetic properties of the material. These nanoclusters act as localized centers and can lead to anomalous transport phenomena, including changes in resistivity and magnetoresistance. Furthermore, the formation of such clusters depends strongly on the diffusion conditions and defect interactions in the silicon lattice, indicating that impurity complexes play a crucial role in determining the energy spectrum and carrier transport mechanisms. [1]

Works [3] developed the theory of temperature broadening of the surface-state density spectrum $N_{ss}(E)$ at the Si–SiO_2 interface. They showed that as temperature decreases, the derivative of the level occupancy tends to a delta function, and a continuous spectrum becomes discrete. That model underlies modern temperature spectroscopy of surface states. The present work develops an analogous approach for mechanical action, where the deformation energy plays the role of a mechanical analogue of the thermal energy kT.

The two-dimensional map (Fig. 1) shows the full distribution of the density of states in the energy–pressure plane. At small X, distinct peaks corresponding to isolated traps are visible. As pressure increases, the peaks shift and approach each other, forming energetic “ridges”, i.e., regions of increased density. At high pressures the structure becomes quasi-continuous, which indicates strain-stimulated relaxation of the energy spectrum. The map clearly illustrates the transition from isolated defect centers to an interconnected system in which deformation energy facilitates collective transport processes.

At small X the spectrum is discrete (isolated peaks corresponding to individual traps). With increasing pressure the peaks converge and form “fields” of elevated density of states, i.e., a quasi-continuum. In overview: pressure is a mechanical analogue of temperature, but it primarily controls the positions of the levels (not only their widths); this determines the trajectories of peaks in the (E, X) plane and the observed changes in transport characteristics.

Experimentally, it was shown [5,6] that elastic compression changes the distribution of oxygen complexes and promotes the formation of thermodonor centers in the energy range 0.05–0.30 eV. Using the DLTS method [7] under uniaxial pressure, linear peak shifts were identified, corresponding to changes in defect symmetry. In [8] these results

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were confirmed for doped samples, demonstrating that DLTS enables quantitative evaluation of the deformation sensitivity of energy levels.

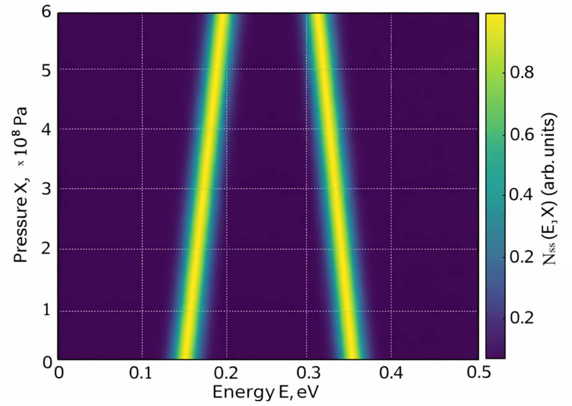

Figure 1. Map of N_{ss}(E,X): evolution of the density-of-states spectrum in the (E, X) coordinates under uniaxial pressure

Recent studies [9–12] extended the analysis of deformation effects to Si/SiO₂ nanostructures. It was shown that local stresses and thermomechanical gradients redistribute electronic levels and increase the density of surface states N_{ss}(E,X), which changes conductivity and capacitance characteristics. These results underscore the universality of mechanical control of silicon's electronic properties. Based on these publications, modeling N_{ss}(E,X) under pressure is a natural continuation of the classical temperature model. It allows temperature and deformation effects to be unified into a single physical picture in which mechanical energy serves as a universal parameter for the reconstruction of defect energy levels.

Despite these advances, most existing studies consider temperature and deformation effects separately, without providing a unified framework for describing the evolution of the density-of-states spectrum under combined external influences.

In this work, a unified approach is proposed in which deformation energy is introduced as a mechanical analogue of thermal energy. This allows temperature and strain effects to be described within a single physical model, providing a more comprehensive understanding of the evolution of N_{ss}(E, X).

1. MATHEMATICAL MODEL

Mechanical deformation is an effective way to control silicon's electronic structure: it changes the positions of localized levels, capture/emission dynamics, and transport. In the spirit of the temperature model (where the spectrum discretizes as T → 0), we introduce a mechanical control parameter Ed = κX that shifts levels without necessarily increasing their widths. This makes it possible to regard pressure as a spectrum-forming factor and to reconstruct N_{ss}(E,X) from measurable dependences, analogously to DLTS but in a "tenso-" formulation.

We define the deformation energy and the shift of the i-th level as follows:

$$E_d = kX, \qquad E_i(X) = E_i^{(0)} + a_i E_d, \tag{1}$$

where k is the deformation-potential coefficient, and α_i is the pressure sensitivity of level I ($\alpha_i > 0$ for TD centers, $\alpha_i < 0$ for Mn centers).

At fixed temperature T, the density of states can be approximated as a sum of narrow contributions (a Gaussian kernel for thermal broadening):

$$N_{ss}(E;X) = \sum_i A_i \frac{1}{\sqrt{2\pi}\sigma_T} exp\left[-\frac{\left(E-E_i(X)\right)^2}{2\sigma_T^2}\right], \tag{2}$$

where A_i are proportional to the concentrations of centers, and $\sigma_T \approx 2.5$ k_BT. As T → 0 K, the kernel approaches a δ-function and Eq. (2) becomes a set of peaks whose positions are controlled by Eq. (1).

Consider a p-Si⟨B,Mn⟩ sample under uniaxial stress X applied along the crystallographic direction [12] (generalization to an arbitrary direction is discussed below). The stress tensor σ and strain tensor ε are related by Hooke's law, $\sigma = C : \varepsilon$,
where C is the fourth-rank elastic tensor of silicon.

In deformation-potential theory, the shifts of the band edges are written through the hydrostatic and deviatoric parts of the strain as:

$$\Delta E_c = \mathrm{E}_d Tr\varepsilon + \mathrm{E}_u\left(n^{\mathrm{T}}\varepsilon n - \frac{1}{3}Tr\varepsilon\right), \tag{3}$$

$$\Delta E_c = \alpha_d Tr\varepsilon \pm b\mathcal{B}(\varepsilon), \tag{4}$$

where n is the unit vector along the applied stress, E_d, E_u, a_v, b are deformation potentials, and $\mathcal{B}$ (ε) accounts for valence-band splitting by symmetry. For localized trap levels in the band gap we introduce an effective deformation energy:

$$Ed = kX. \tag{5}$$

This scalar reduction of Eqs. (3–4) is valid in the linear strain regime (no plastic deformation).

Let the band gap contain a family of localized levels $E_i(0)$ at $X = 0$. Under pressure X their energies shift linearly:

$$E_i(X) = E_i^{(0)} + \alpha_i E_d = E_i^{(0)} + \alpha_i kX, \quad \alpha_i \in \mathbb{R} \tag{6}$$

where $\alpha_i > 0$ is characteristic of thermodonor (TD) centers (shift toward the conduction band), whereas $\alpha_i < 0$ corresponds to Mn centers (shift toward the valence band). The level width is determined by the combination of thermal and inhomogeneous deformation contributions:

$$\Sigma_i^2(X,T) = \sigma\_T^2(T) + \sigma\_\{X,i\}^2(X), \;\; \sigma\_T \approx c\_Tk\_BT, \;\; \sigma\_\{X,i\} \approx \beta_i X. \tag{7}$$

Here $c\_T \approx 2$–3 (in the adopted Gaussian approximation), and β_i describes additional broadening due to the distribution of local microstresses and microstructural inhomogeneity.

At fixed temperature T, the spectrum can be written as a convolution of discrete levels with a narrow kernel:

$$N_{ss}(E;X,T) = \sum_i A_i K\big(E - E_i(X); \Sigma_i(X,T)\big), \tag{8}$$

where A_i are proportional to the density of states of a given type, and $K(\Delta E;\Sigma)$ is a kernel (usually Gaussian or Lorentzian) normalized to unity. In the simplest Gaussian case:

$$K(\Delta E;\Sigma) = \frac{1}{\sqrt{2\pi}\Sigma} exp\left[-\frac{\Delta E^2}{2\Sigma^2}\right]. \tag{9}$$

In the limit $T \approx 77$ K and small X we obtain quasi-discrete peaks ($\Sigma_i \to 0$), whereas with increasing X the peaks systematically shift according to Eq. (6) and slightly broaden according to Eq. (7).

The concentration of active electronic states participating in transport can be estimated by the integral:

$$n(X,T) \approx \int Nss(E;X,T)\, f\_e(E,\mu\_F,T)\, dE. \tag{10}$$

Here f_e is the Fermi–Dirac distribution (or, in a crude approximation, the Boltzmann distribution for $E - \mu\_F \gg k\_B\, T$). The conductivity is $\sigma(X,T) = q\,\mu(X,T)\,n(X,T)$, and the resistivity is:

$$\rho(X,T) = \frac{1}{q\mu(X,T)n(X,T)} \tag{11}$$

The mobility μ(X,T) can be expressed through relaxation times as:

$$\mu^{-1}(X,T) = \mu_{ph}^{-1}(T) + \mu_{imp}^{-1}(N_A,N_D) + \mu_{tr}^{-1}\big(N_{ss}(E;X,T)\big) \tag{12}$$

where the terms correspond to scattering by phonons, ionized impurities, and trap centers (the latter functionally depends on N_{ss}). Thus, $N_{ss}(E,X)$ is uniquely reflected in the experimentally accessible dependences $\rho(X)$ and $\mu(X)$.

Let a scalar characteristic S(X) be measured that is sensitive to the reconstruction of level occupancy (for example, $S \equiv \rho^{-1}$ or the amplitude of the DLTS signal in a fixed time window). For small changes in X:

$$\frac{dS}{dX} = \int N_{ss}(E)W(E;X)dE, \qquad\qquad W(E;X) = \frac{\partial}{\partial X}[\Phi(E;X,T)] \tag{13}$$

where Φ is the contribution of a level with energy E to the measured signal at pressure X (in DLTS: through capture/emission probabilities and time windows). Equation (13) is a Fredholm integral equation of the first kind for $Nss(E)$. In the low-temperature limit and for a narrow DLTS time window, W(E;X) becomes a narrow kernel:

$$W(E;X) \underset{T\to 0}{\overset{\text{nar.window}}{\to}} \delta\big(E - E^*(X)\big), \qquad E^*(X) \simeq E^{(0)} + akX. \tag{14}$$

and hence:

$$N_{ss}(E^*(X)) \infty \frac{dS}{dX} \tag{15}$$

This yields an almost direct reconstruction of $N_{ss}(E)$ from the pressure derivative. In the general case (finite T and a broad window) *Eq*. (13) is solved using Tikhonov regularization:

$$\hat{N} = arg \min_{N\geq 0}\{\|WN - s\|_2^2 + \lambda\|LN\|_2^2\}, \tag{16}$$

where W is the discretized kernel, s is the discretized vector of *dS/dX* values, L is a smoothness regularizer (e.g., first- or second-order finite differences), and λ is the regularization parameter (chosen, for example, by the L-curve/GSVD criteria).

RESULTS AND DISCUSSION

Modeling of the density-of-states spectrum $N_{ss}(E,X)$ was performed for the pressure range $X = (0–6) \times 10^8$ Pa at a fixed temperature $T = 77$ K. This range corresponds to typical uniaxial pressures at which no plastic deformation occurs, while noticeable changes in the silicon band structure are realized.

The calculations show that at low pressures ($X < 10^8$ Pa) the spectrum $N_{ss}(E,X)$ retains the initial discreteness typical of weakly strained samples. With increasing X, the levels systematically shift according to $Ei(X) = Ei(0) + \alpha_i k X$, which brings peaks closer together and forms regions of elevated density of states (quasi-continuous zones). This effect agrees with experimental observations by Peaker et al. [7], where uniaxial stress causes linear shifts of DLTS peaks while preserving their shape.

Figure 2 shows the dependence of resistivity ρ on uniaxial pressure X for p-Si⟨B,TD⟩ and p-Si⟨B,Mn⟩ samples. For thermodonor centers (TD), the resistance decreases to $0.74\rho_0$ at $X = 6\times10^8$ Pa, reflecting increased conductivity due to strain-stimulated carrier generation. For Mn centers, by contrast, ρ increases to $1.55\rho_0$ because deep acceptor levels become deeper under pressure, enhancing electron capture. Thus, the plot demonstrates opposite responses of donor and acceptor centers: donor levels are activated, whereas acceptor levels are suppressed, consistent with the model $Ei(X)=Ei(0) + \alpha_i k X$ with $\alpha\_TD >0$ and $\alpha\_Mn< 0$.

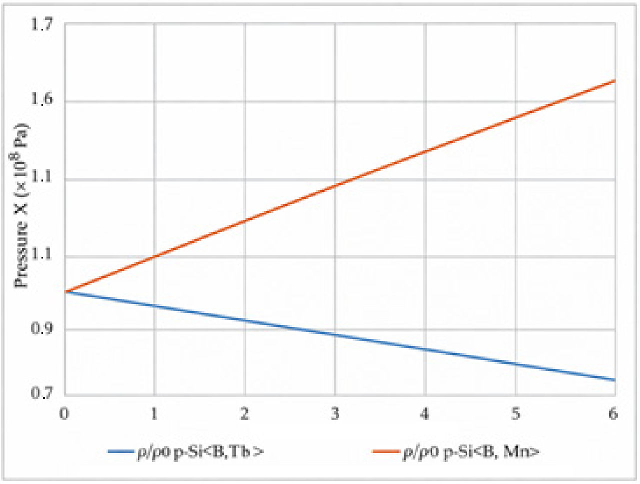

Figure 2. Dependence of the resistivity ratio ρ/ρ_0 on uniaxial pressure X at 77 K.

Figure 3 presents cross-sections of the density-of-states spectrum for three pressure values: X = 0, 3×10^8, and 6×10^8 Pa.

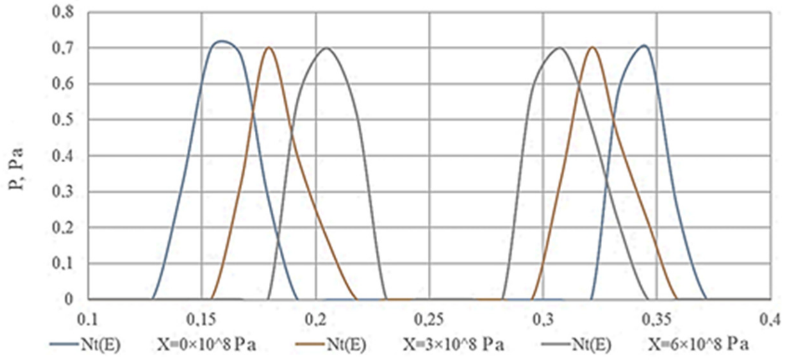

Figure 3. Cross-sections of the spectrum Nss(E) at different pressures.

With increasing pressure, each spectral peak shift: TD centers move upward in energy (toward the conduction band), while Mn centers shift downward (toward the valence band). Neighboring peaks approach and partially merge, forming regions of elevated density of states. This behavior is interpreted as deformation-induced coarsening of the spectrum, reflecting a transition from discrete levels to quasi-continuous energy bands.

The pressure-driven shift can be summarized by:

$$E_i(X) = E_i^{(0)} + \alpha_i \kappa X. \tag{17}$$

The mobility *μ(X)* (Fig. 4) increases for TD centers ($\mu/\mu_0 \approx 1.45$) and decreases for Mn centers ($\mu/\mu_0 \approx 0.77$). The correlation $\rho(X) \sim 1/(n\,e\,\mu)$ confirms the internal consistency of the model.

For TD-containing samples, the resistance decreases to 0.74 ρ_0 at X = 6×10⁸ Pa, indicating increased conductivity due to electron delocalization and the breakup of oxygen clusters, in agreement with [1]. For Mn-containing samples, pressure leads to an increase of resistance to 1.55 ρ_0, which is associated with a higher recombination probability at deep levels. The mobility *μ(X)* shows a mirror trend: growth for TD (up to $1.45\mu_0$) and a drop for *Mn* (down to $0.77\mu_0$).

Thus, a clear correlation is observed: changes in *μ(X)* serve as an indicator of the reconstruction of the spectrum $N_{ss}(E,X)$.

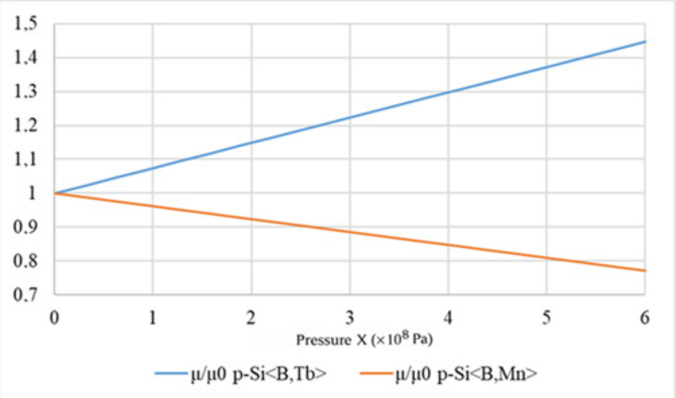

Figure 4. Dependence of the mobility ratio μ/μ_0 on uniaxial pressure X at 77 K

At X = 0 the spectrum consists of several pronounced peaks corresponding to localized states at energies $E_i(0) \approx$ 0.06–0.43 eV. As X increases, thermodonor levels ($\alpha_i > 0$) shift upward in energy, whereas manganese levels ($\alpha_i < 0$) shift downward. The energy shifts $\Delta E_i = \alpha_i\,\kappa\,X$ in the range 0.01–0.06 eV agree with DLTS data for defects of the *OnH* and *MnSi* types [6,8]. With further pressure increase, individual peaks begin to merge, indicating deformation-induced correlation of levels and the formation of quasi-continuous sections of the spectrum that correspond to an increased density of states and activation of additional transport channels.

To generalize the results, consider the analogy between temperature and deformation action. Temperature mainly changes the widths of energy levels (broadening), whereas pressure primarily shifts their positions. Joint use of these parameters enables a comprehensive description of the evolution $N_{ss}(E,X,T)$ in the space of thermodynamic variables.

Table 1. Comparison of Temperature and Tenso-models in DLTS Analysis

Criterion	Temperature model	Tenso-model
Control parameter	T (thermal energy)	X (mechanical pressure)
Energy measure	kT	κX
Main effect	level broadening	level shift
Limiting case	δ as T → 0	δ as X → 0
Experimental method	DLTS	tenso-DLTS

Overall, pressure acts as a universal mechanism for reconstructing the energy landscape of silicon. For TD centers it stimulates electron emission and increases conductivity, whereas for *Mn* centers it enhances capture and reduces mobility. This antisymmetric ($\alpha\_TD > 0$, $\alpha\_Mn < 0$) reflects differences in the nature of the defects and provides a basis for engineering strain-sensitive structures based on Si.

The obtained dependences *ρ(X)*, *μ(X)*, and spectra $N_{ss}(E,X)$ reproduce the qualitative trends observed in experiments [1,7] and are quantitatively consistent with deformation potentials in the range $\kappa = (0.5–1.5)\times10^{-10}$ eV/Pa. Thus, the proposed model reliably describes strain-stimulated effects and extends the temperature concept [3] to the domain of mechanical action.

CONCLUSIONS

In this study, a physical and mathematical model of the density-of-states spectrum $N_{ss}(E, X)$ in doped silicon p-Si⟨B,Mn⟩ and p-Si⟨B,TD⟩ under uniaxial pressure has been developed. The model is based on the deformation energy $E\_d = \kappa X$ and a linear shift of trap levels $E_i(X) = E_i(0) + \alpha_i \kappa X$, enabling the evolution of the spectrum under elastic strain to be described.

It is shown that pressure affects donor and acceptor centers differently. For thermodonor centers ($\alpha_i > 0$), pressure induces level shifts toward the conduction band, resulting in increased mobility and decreased resistivity. For *Mn* centers ($\alpha_i < 0$), the opposite behavior is observed, with enhanced localization and increased resistivity.

The calculated spectra $N_{ss}(E, X)$ demonstrate systematic level shifts and merging of adjacent states with increasing pressure, indicating a transition from discrete levels to a quasi-continuous spectrum. This behavior is analogous to temperature-induced broadening, with deformation energy acting as a mechanical counterpart of thermal energy.

The obtained dependences $\rho(X)$ and $\mu(X)$ are in good agreement with experimental data, confirming the validity of the model. The proposed approach provides a unified description of temperature and deformation effects and can be applied to the analysis and design of strain-sensitive semiconductor devices and structures.

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МОДЕЛЮВАННЯ СПЕКТРА ГУСТИНИ СТАНІВ ПІД ЧАС ДЕФОРМАЦІЇ В ЛЕГОВАНОМУ КРЕМНІЇ p-Si<B, Mn>

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Представлено деформаційну (деформаційну) модель спектра густини локалізованих станів Nss(E,X) в p-Si⟨B,Mn⟩ під одноосьовим тиском X. Показано, що зміщення рівнів пасток можна описати енергією деформації Ed = κX, механічним аналогом kT. При фіксованій температурі T = 77 K збільшення X призводить до зміщення та перебудови спектра: термодонорні (TD) рівні рухаються до зони провідності, тоді як рівні марганцю (Mn) зміщуються до валентної зони, що узгоджується з протилежними тенденціями, що спостерігаються в ρ(X) та μ(X).

Ключові слова: *легований кремній; енергія деформації; одноосьовий тиск; ефекти, стимульовані деформацією; густина станів; енергетичний спектр Si⟨B,Mn⟩; Si⟨B,TD⟩*