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DETERMINATION OF THE ENERGY SPECTRUM OF THE DENSITY OF STATES UNDER UNIAXIAL PRESSURE

M.A. Rakhmanov[1], I.G. Tursunov[1], O.O. Mamatkarimov[2], N.Yu. Sharibaev[2], S.S. Sharipbaev[2]*
[1]*Chirchik State Pedagogical University, 111702, Tashkent, Uzbekistan*
[2]*Department of Energy Engineering, Namangan State Technical University, Namangan, Uzbekistan*
**Corresponding Author email: sharipbaev1999@gmail.com*
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This paper considers the influence of hydrostatic pressure on the energy spectrum of the density of localized states in doped silicon n-Si, n-Si⟨Ni⟩ and p-Si⟨B,Mn⟩. Based on the experimental dependence of the relative resistivity ρ_P/ρ_0 on pressure, a model is constructed in which pressure enters via the deformation energy Ed = κP, yielding a linear shift of the trap levels $E_i(P) = E_i(0)+\alpha_i Ed$. It is shown that for different impurity centers (Mn, Ni) the deformation sensitivity of the levels differs in both sign and magnitude, which is manifested in qualitatively different behavior of $\rho_P/\rho_0(P)$. A procedure is proposed for reconstructing the relative electron concentration $N(P)/N_0$ and the associated spectrum $N_{ss}(E,P)$ from the experimental $\rho_P/\rho_0(P)$ curves. A comparison is made with the conventional temperature DLTS model, and the possibility of using a "tenso-DLTS" approach to identify donor and acceptor centers, their deformation potentials and symmetry is substantiated. The results demonstrate that hydrostatic pressure is not only an external perturbation, but also an effective spectrum-forming parameter for controlling the electronic properties of doped silicon.
Keywords: *Doped silicon; Hydrostatic pressure; Deformation energy; Density-of-states spectrum; Localized levels; Tenso-DLTS; Resistivity; n-Si⟨Ni⟩; p-Si⟨B,Mn⟩; Transition-metal impurity centers*
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INTRODUCTION

The study of the influence of mechanical pressure on energy levels in silicon has been actively developing for the past several decades. In the literature, several directions can be distinguished that are directly related to the problem of determining the spectrum $N_{ss}(E,X)$.

The first experiments on recording DLTS spectra under uniaxial stress showed that mechanical stress causes splitting and linear shifts of trap peaks, thereby enabling the determination of their symmetry and pressure sensitivity [1–4]. These works laid the foundation of a method in which the derivative with respect to stress X is measured and the distribution $N_{ss}(E)$ is reconstructed by analogy with temperature DLTS.

A number of studies [4–7] have shown that mechanical stresses, including hydrostatic pressure, accelerate the formation of oxygen thermal donors and change the concentration of oxygen clusters. This explains the decrease in resistivity $\rho(X)$ and the increase in mobility $\mu(X)$ in p-Si⟨B,TD⟩ samples with increasing pressure. Such effects are interpreted through changes in the band structure and charge redistribution between heavy and light bands.

Modern theoretical and experimental works [8–10] show that mechanical stress leads to the depassivation of interface centers, distortion of Si–O bonds, and an increase in the density of surface states. As the pressure increases, "silent" traps are activated, thereby confirming the formation of a new density of states, Nss(E,X), at the interface.

Studies of piezoresistance [11, 12] demonstrate that the combination of defects and mechanical stress radically changes charge transport in silicon, especially in SOI structures. Changes in $\rho(X)$ and $\mu(X)$ correlate with a restructuring of the DOS, and their analysis enables quantitative evaluation of the parameters α_i and κ in models of tenso-stimulated effects. All of these works confirm that mechanical pressure acts not only as an external parameter but also as a spectrum-forming factor that changes the structure of localized states. It is precisely on this principle that the model $N_{ss}(E,X)$ proposed in the present article is built; it develops the temperature concept of Gulyamov and Sharibaev [13] and is consistent with subsequent experiments [14].

In recent decades, studies of the influence of external factors, such as temperature, pressure, irradiation, and doping, on the electronic properties of semiconductors have become particularly important in connection with the development of nanoelectronics and sensor technologies. One of the key directions is the study of the energy spectrum of the density of states (DOS) and the mechanisms of its change under mechanical deformations and uniaxial pressure.

Traditionally, analysis of the density of states has been performed via temperature dependences, as is clearly illustrated in [13]. The authors showed that as the temperature decreases, the function $\partial\rho(E,E_0,T)/\partial E_0$ approaches the Dirac δ-function, and the continuous spectrum Nss(E,T) gradually breaks into discrete peaks. However, temperature is not the only factor affecting the DOS spectrum: external uniaxial pressure can cause energy-level shifts of a similar nature, changing carrier localization and the structure of the potential landscape [14].

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The aim of this work is to develop a method for reconstructing the energy spectrum of localized states $N_{ss}(E,X)$ in doped silicon under mechanical (hydrostatic or uniaxial) pressure, based on experimental dependences of relative resistivity. The study also aims to establish a physical analogy between temperature- and pressure-induced transformations of the density-of-states spectrum.

MATHEMATICAL MODEL

When considering the influence of external pressure on the electronic properties of silicon, it is convenient to introduce the concept of deformation energy E_d, which quantitatively characterizes the change in the energy landscape under elastic compression of the crystal:

$$E_d = \kappa X, \tag{1}$$

where X is the external uniaxial (or hydrostatic) pressure and κ is the deformation potential coefficient (eV/Pa), which depends on the elastic constants and the crystal orientation.

Introducing this quantity makes it possible to treat pressure as an analogue of temperature in the traditional model [13], where a change in temperature leads to broadening and shifting of energy levels. In the case of pressure, this effect is caused by elastic shifts of the band structure and changes in electron localization in the region of defects.

Each localized level in the band gap shifts according to a linear law

$$E_i(X) = E_i(0) + \alpha_i E_d, \tag{2}$$

where $E_i(0)$ is the level energy without deformation and α_i is the sensitivity coefficient of the level to pressure (the sign $\alpha_i > 0$ corresponds to a shift towards the conduction band, and $\alpha_i < 0$ to a shift towards the valence band).

Thus, under pressure the trap structure changes not only in terms of energy position but also in terms of the density of states $N_{ss}(E,X)$. This reflects the physical picture of carrier redistribution and the onset of tenso-stimulated electron generation from localized centers.

In the most general form, the probability of releasing an electron from a state with energy E_i can be written as

$$\rho(E_i, E_d) = 1 - exp\left[-\frac{t_0}{\tau(E_i)}F(E_d)\right], \tag{3}$$

where t_0 is the characteristic measurement time, $\tau(E_i)$ is the relaxation time of the level, and $F(E_d)$ is a function describing the increase in probability with increasing pressure (in the simplest case, $F(E_d) = \exp(E_d/E_a)$, where E_a is the activation energy).

Differentiating Eq. (3) with respect to E_d gives the sensitivity function

$$\frac{\partial\rho(E_i,E_d)}{\partial E_d} = \frac{t_0}{\tau(E_i)}\frac{dF(E_d)}{dE_d}\exp\left[-\frac{t_0}{\tau(E_i)}F(E_d)\right]. \tag{4}$$

This function is close in shape to a Gaussian and, in the limit $E_d \to 0$, is equivalent to the Dirac δ-function. This means that at low temperatures and small pressures, the response of the system becomes discrete, which physically corresponds to the appearance of isolated trap centers.

Figure 1 illustrates this behavior: as the effective width of the kernel in deformation energy decreases, the function becomes sharper and approaches the δ-function.

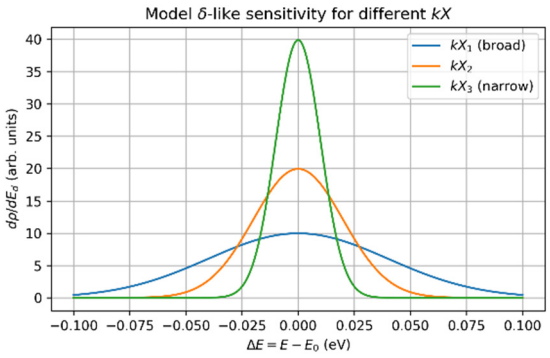

Figure 1. Model δ-like sensitivity function ∂ρ/∂Ed for different values of the effective parameter kX (kernel width)

Determination of the density of states

The density of states that depends on pressure can be described by the integral relation

$$N(E_d) = \int N_{ss}(E)\rho(E,E_d)dE \tag{5}$$

where $N_{ss}(E)$ is the true distribution of levels over energy and $\rho(E,E_d)$ is the probability of their activation at a given pressure.

Differentiating Eq. (5) with respect to E_d yields

$$\frac{dN(E_d)}{dE_d} = \int N_{ss}(E)\frac{\partial\rho(E,E_d)}{\partial E_d}dE. \tag{6}$$

At low temperatures and small E_d, where

$$\frac{\partial\rho(E,E_d)}{\partial E_d} \to \delta(E - E_0), \tag{7}$$

the measured dependence dN/dE_d is directly proportional to $N_{ss}(E)$.

As the width decreases, the function becomes narrower and approaches the Dirac δ-function.

In other words, by measuring currents or signals that depend on pressure (analogous to temperature DLTS spectra), one can experimentally reconstruct the distribution of trap levels over energy:

$$N_{ss}(E_0) \infty \frac{dN(E_d)}{dE_d}\Big|_{E_d \to 0}. \tag{8}$$

In the real case of finite temperature and nonlinear behavior of the levels, the reconstruction of $N_{ss}(E)$ is carried out numerically. For this purpose, a smoothing kernel (for example, a Gaussian) is introduced and the approximation

$$N_{ss}(E,X) \approx \sum_i A_i K_T\big(E - E_i(X)\big) \tag{9}$$

is used, where A_i is the amplitude (concentration of the corresponding center), and $K_T(E)$ is a broadening function (which tends to a δ-function as $T \to 0$).

Figure 2 schematically shows the temperature evolution of the spectrum $N_{ss}(E,T)$: as T decreases, the peaks of the spectrum become narrower and approach a discrete set of levels. By analogy, deformation energy E_d acts as an additional control parameter.

This representation makes it possible to construct a map of the evolution of the spectrum $N_{ss}(E,X)$ at different pressures and to determine the nature of the level shift:

$$\Delta E_i = \alpha_i \kappa X. \tag{10}$$

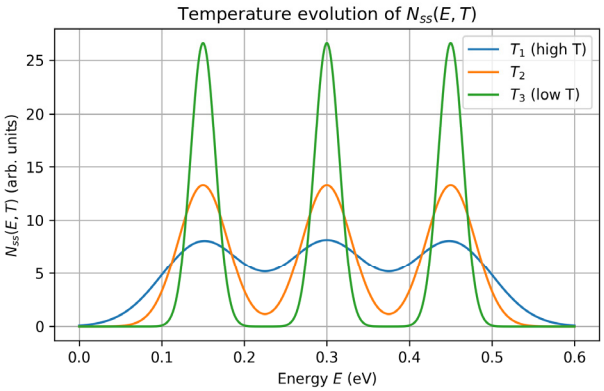

Figure 2. Schematic temperature evolution of the spectrum of the density of states Nss(E,T)

At high temperature, the peaks are broad and partially overlap; at intermediate temperature, the structure becomes more pronounced; at low temperature, the spectrum approaches a set of discrete levels. By analogy, the deformation energy E_d serves as an additional control parameter.

Physical interpretation

An increase in pressure increases the deformation energy E_d, which leads to:

- for thermal donor (TD) centers: an upward shift of the levels towards the conduction band and enhanced electron generation (decrease in ρ, increase in μ);
- for Mn centers: a downward shift towards the valence band and an increase in resistivity (decrease in mobility). Thus, the functions $\rho(X)$ and $\mu(X)$ reflect carrier redistribution, while the map $N_{ss}(E,X)$ reflects the energy

dynamics of localized states. Joint analysis of these dependences makes it possible to determine not only the deformation parameters κ and α_i, but also to identify active defect centers in the bulk and at the surface of the semiconductor.

Results of Modeling and Discussion

The novelty of this work lies in the development of a unified approach to analyzing the energy spectrum of localized states in doped silicon under mechanical pressure, based on the introduction of deformation energy as an analog of thermal energy. Within this framework, a method is proposed to reconstruct the density-of-states spectrum from experimentally measured pressure-dependent resistivity, thereby enabling a direct link between macroscopic electrical characteristics and the underlying energy distribution of defect states. In contrast to conventional temperature-based DLTS techniques, the presented approach extends the analysis to pressure-induced effects and demonstrates that mechanical deformation can serve as an independent and effective parameter for controlling and diagnosing the electronic structure of semiconductor materials.

The calculations were carried out at $T = 77$ K and $X = 0...6\times10^8$ Pa. The model includes several levels in the range 0.1–0.45 eV with different α_i. Pressure acts as a universal parameter that determines the redistribution of trap states. Typical parameter values are $\kappa = 1.0\times10^{-10}$ eV/Pa, $E_i(0) \in [0.06,0.45]$eV. Table 1 compares the temperature model and the tenso-model.

Table 1. Comparison of temperature and tenso models.

Parameter	Temperature model	Tenso-model
Control quantity	T (thermal energy)	X (mechanical pressure)
Energy scale	kT	κX
Nature of effect	Thermal broadening	Deformation-induced shift
Limiting behavior	δ-function as T → 0	δ-function as X → 0
Experimental form	DLTS	Tenso-DLTS

Both models describe a transition from a continuous to a discrete spectrum. Temperature changes the width of the levels; pressure changes their position. The calculations show a linear shift

$$\Delta E_i = \alpha_i \kappa X, \tag{11}$$

which makes it possible to estimate κ and construct a map of defect centers.

The behavior of the relative resistivity $\rho(X)/\rho_0$ for p-Si⟨B,TD⟩ and p-Si⟨B,Mn⟩ is illustrated in Fig. 3. For p-Si⟨B,TD⟩ the resistivity decreases from $\rho/\rho_0 \approx 1$ to ~ 0.74 as pressure increases, which corresponds to an increase in carrier concentration and mobility. For p-Si⟨B,Mn⟩ the resistivity increases up to $\sim 1.55\rho_0$, which indicates enhanced localization and growth of the fluctuation potential.

In the case of n-Si⟨Ni⟩, experimental data for ρ_p/ρ_0 show a two-step increase $1 \rightarrow 9 \rightarrow 15$, which corresponds to a two-step decrease in $N(P)/N_0$ ($1 \rightarrow 0.11 \rightarrow 0.07$). This indicates the presence of at least two groups of Ni-related centers with different deformation sensitivities, and the corresponding dependence can be modeled as

$$\frac{N_3(P)}{N_0} \approx \left[1 + \frac{A_1}{1+\exp\left(-(P-P_1)/\Delta P_1\right)} + \frac{A_2}{1+\exp\left(-(P-P_2)/\Delta P_2\right)}\right] \tag{12}$$

where A_1 and A_2 are the amplitudes of the steps, and P_1, P_2 are the characteristic pressures for activation of each group of centers. Such behavior is a direct graphical confirmation of the complex multi-component nature of the energy spectrum of Ni-related levels. For thermal donor centers (TD), pressure stimulates electron delocalization and a decrease in resistivity, as illustrated in Figure 3.

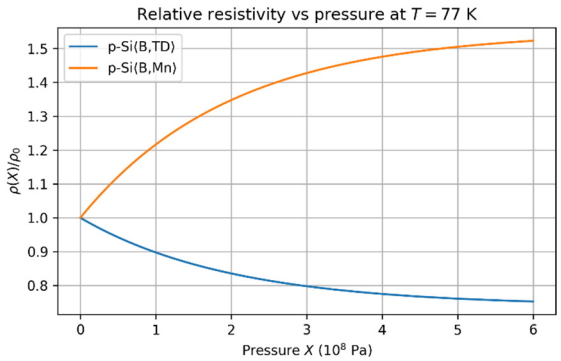

Figure 3. Calculated dependences of relative resistivity ρ(X)/ρ0 on uniaxial pressure X at T = 77 K for p-Si⟨B,TD⟩ (decreasing curve) and p-Si⟨B,Mn⟩ (increasing curve)

CONCLUSIONS

The study carried out extends the classical temperature model [13] and demonstrates that uniaxial (or hydrostatic) pressure can serve as an equivalent control parameter in forming the energy spectrum of the density of states in silicon. The introduced deformation energy $E_d = \kappa X$ describes a mechanical analogue of the thermal energy kT, and the transition from a continuous to a discrete spectrum with increasing pressure fully corresponds to the behavior of the system upon cooling.

It is shown that a change in external pressure causes not only a shift of energy levels but also their redistribution: as X increases, individual trap states merge into quasi-continuous bands, forming a deformation-induced continuum. Quantitatively, the model predicts a deformation coefficient κ on the order of 1.0×10^{-10} eV/Pa, while the relative resistivity changes from $\rho/\rho_0 \approx 1$ to ~0.74 for thermal donor centers and increases up to $\sim1.55\rho_0$ for Mn-related centers. These results demonstrate the significant role of mechanical deformation in modifying the energy spectrum of localized states.

For TD centers, pressure leads to a decrease in resistivity (increase in conductivity); for Mn centers, to an increase in resistivity. for manganese centers (Mn) it leads to an increase in recombination losses and a rise in ρ(X). These opposite trends are reflected in the sign of the sensitivity coefficient αi and characterize the difference in the mechanisms of interaction between defects and the lattice.

A linear dependence $\Delta E_i = \alpha_i \kappa X$ is established, which makes it possible, using the spectrum $N_{ss}(E,X)$, to determine the deformation potentials κ and the type of active centers. Thus, the map $N_{ss}(E,X)$ serves as a direct indicator of the internal structure of defect complexes.

The developed tenso-DLTS methodology can be used for non-destructive analysis of the defect structure of silicon substrates and Si–SiO_2 interfaces at low temperatures, as well as for monitoring the stability of sensitive elements in microsystem electronics. The proposed model opens the way to the creation of tenso-sensitive sensors, MEMS elements and micromechanical structures in which mechanical pressure is used as a tuning parameter for the electronic properties of the material.

Overall, the results obtained show that mechanical deformation plays a role as fundamental in restructuring the energy spectrum as temperature and can be regarded as a new tool for controlled modification of electronic states. This approach forms the basis for the development of "tenso-spectroscopy of states" — a new diagnostic direction in semiconductor physics and technology.

ORCID

N.Yu. Sharibaev, https://orcid.org/0009-0000-3482-5092; **O.O. Mamatkarimov,** https://orcid.org/0009-0005-9501-6295
M.A. Rakhmanov, https://orcid.org/0009-0007-4611-7641; **I.G. Tursunov,** https://orcid.org/0000-0002-5094-6705
S.S. Sharipbaev, https://orcid.org/0009-0009-2269-7711

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ВИЗНАЧЕННЯ ЕНЕРГЕТИЧНОГО СПЕКТРА ГУСТИНИ СТАНІВ ПІД ОДНООСНИМ ТИСКОМ

М.А. Рахманов[1], І.Г. Турсунов[1], О.О. Маматкарімов[2], Н.Ю. Шарібаєв[2], С.С. Шаріпбаєв[2]
[1]Чирчикський державний педагогічний університет, 111702, Ташкент, Узбекистан
[2]Кафедра енергетичного машинобудування, Наманганський державний технічний університет, Наманган, Узбекистан

У цій роботі розглядається вплив гідростатичного тиску на енергетичний спектр густини локалізованих станів у легованому кремнії n-Si, n-Si⟨Ni⟩ та p-Si⟨B,Mn⟩. На основі експериментальної залежності відносного опору ρp/ρ0 від тиску побудовано модель, в якій тиск входить через енергію деформації Ed = κP, що призводить до лінійного зсуву рівнів пасток $E_i(P) = E_i(0)+\alpha_i Ed$. Показано, що для різних домішкових центрів (Mn, Ni) деформаційна чутливість рівнів відрізняється як за знаком, так і за величиною, що проявляється в якісно різній поведінці $\rho_p/\rho_0(P)$. Запропоновано процедуру реконструкції відносної концентрації електронів N(P)/N0 та пов'язаного з нею спектру $N_{ss}(E,P)$ з експериментальних кривих ρp/ρ0(P). Проведено порівняння зі звичайною температурною моделлю DLTS та обґрунтовано можливість використання підходу «тензо-DLTS» для ідентифікації донорних та акцепторних центрів, їх деформаційних потенціалів та симетрії. Результати демонструють, що гідростатичний тиск є не лише зовнішнім збуренням, але й ефективним параметром формування спектра для контролю електронних властивостей легованого кремнію.

Ключові слова: *легований кремній; гідростатичний тиск; енергія деформації; спектр густини станів; локалізовані рівні; тензо-DLTS; питомий опір; n-Si⟨Ni⟩; p-Si⟨B,Mn⟩; домішкові центри перехідних металів*