DEEP-LEVEL KINETICS AND THERMOMECHANICAL WAVE PHENOMENA IN COMPENSATED SILICON UNDER PULSED HYDROSTATIC PRESSURE

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Abstract: This work investigates the fundamental mechanisms governing the transient piezoresistive response of nickel-compensated silicon (n-Si:P,Ni and p-Si:P,Ni) under pulsed hydrostatic pressure. The primary goal is to separate and analyze the static deformational, thermal, and kinetic-relaxation components of the conductivity change observed during and after a rapid pressure pulse. We combine a developed theoretical model of thermomechanical wave processes in the pressure-transmitting fluid with experimental measurements of current kinetics. The theoretical analysis demonstrates that high loading rates generate a non-stationary thermal field, leading to wave-like heat propagation. Experimentally, we observe a pronounced relaxation transient in compensated samples: after the pressure reaches its maximum amplitude of 0.5 GPa, the current continues to increase for several seconds, peaks, and then slowly decays to a steady-state value. A key finding is that the amplitude of this transient significantly exceeds the response caused by pure, isobaric heating of the sample to the same temperature, proving the existence of a pressure-specific, non-equilibrium ionization mechanism beyond simple adiabatic heating. Furthermore, the relaxation magnitude strongly depends on the compensation degree and is more prominent in n-type samples than in p-type ones, indicating the role of carrier type and lattice coupling. The main conclusion is that the dynamic tensoeffect in semiconductors with deep levels is a complex superposition of an instantaneous pressure-induced shift of electronic levels, a transient thermodeformational excitation, and a slow relaxation governed by the kinetics of deep-level occupancy.

Introduction

Semiconductors incorporating deep-level impurities exhibit remarkable sensitivity to external perturbations due to the metastable occupancy of these localized states [1]. Hydrostatic pressure serves as a powerful, defect-free tool to modify the electronic structure, directly shifting energy levels relative to band edges [3]. However, under dynamic (pulsed) loading, the interpretation of electrical measurements becomes complex due to inseparable thermal and deformational contributions [2]. The adiabatic

compression of the pressure medium induces transient heating, while the rapid lattice deformation can drive the deep-level system out of equilibrium. Previous studies have attributed dynamic conductivity changes primarily to this adiabatic heating [2]. Yet, detailed kinetics—such as the continued evolution of conductivity after pressure stabilization—point to more intricate processes involving the finite response time of deep centers and possible thermomechanical wave phenomena. This work aims to elucidate these mechanisms by constructing a detailed theoretical framework for heat and charge carrier dynamics under pulsed pressure and by performing kinetic measurements on nickel-compensated silicon with varying compensation degrees. We seek to quantitatively separate the static, thermal, and kinetic-relaxation components of the piezoresistive response.

Theoretical Framework

Adiabatic Heating and Non-Stationary Thermal Transport

The fundamental temperature change in a fluid under adiabatic compression is given by the thermodynamic relation:

$$dT = \frac{\alpha T}{\rho c_P} dP$$

where α is the coefficient of thermal expansion, ρ is density, c_P is specific heat capacity, and T is temperature. For a finite pressure step ΔP, the idealized temperature rise is

$$\Delta T_{ad} = \frac{\alpha T}{\rho c_P} \Delta P.$$

However, in a real experimental geometry with finite pressure rise time t_r, heat conduction occurs concurrently. The general non-stationary heat equation for the fluid (in one dimension, no internal sources) is:

$$\frac{\partial T}{\partial t} = \frac{\chi}{\rho c_P} \frac{\partial^2 T}{\partial x^2}$$

During compression, T is a function of pressure P(t). Applying the chain rule:

$$\frac{\partial T}{\partial t} = \frac{dT}{dP} \frac{\partial P}{\partial t}$$

Substituting the adiabatic derivative $\frac{dT}{dP} = \frac{\alpha T}{\rho c_P}$ and defining the pressure rise rate $v_p = \partial P / \partial t$, we obtain:

$$v_p \frac{\alpha T}{\rho c_P} = \frac{\chi}{\rho c_P} \frac{\partial^2 T}{\partial x^2}$$

Simplifying yields a Helmholtz-type equation describing the temperature field under dynamic compression:

$$\frac{\partial^2 T}{\partial x^2} - \frac{\alpha v_p}{\chi} T = 0$$

Defining $k^2 \equiv \alpha v_p/\chi$, the solution is exponential, $T(x) \propto \exp(\pm kx)$. The parameter k has dimensions of inverse length and can be interpreted as a wave number associated with the thermal disturbance:

$$k = \sqrt{\frac{\alpha v_p}{\chi}} = \frac{2\pi}{\lambda}$$

where $\lambda = 2\pi\sqrt{\chi/(\alpha v_p)}$ is a characteristic thermal wavelength. This formalism reveals that at high loading rates (v_p > 0), the thermal front propagates as a damped wave rather than by pure diffusion. In the static limit $(v_p \to 0), \lambda \to \infty$, recovering the isothermal condition.

Kinetics of Deep-Level Ionization under Concurrent Pressure and Temperature Transients

The electrical conductivity σ of compensated silicon is $\sigma = e\, n\, \mu$, where the free electron concentration n is determined by the ionization equilibrium of the deep nickel acceptors. The occupancy of the deep level is governed by the rate equation [4]. Let N_A be the total nickel concentration and N_A^- the concentration of ionized (negatively charged) acceptors. The net rate of ionization is:

$$\frac{dN_A^-}{dt} = e_n(T,P)(N_A - N_A^-) - c_n(T), n, N_A^-$$

Here, $e_n(T,P)$ is the emission rate of electrons from the level to the conduction band, and $c_n(T)$ is the electron capture coefficient. The emission rate has an Arrhenius dependence on temperature and a pressure dependence through the level's activation energy $E_a(P)$:

$$e_n(T,P) \propto \exp\left(-\frac{E_a(P)}{k_B T}\right)$$

A linear pressure shift is assumed: $E_a(P) = E_a(0) - \beta P$, with $\beta > 0$ [5].

During and after a pressure pulse, both T(t) and P(t) change. The observed current transient $I(t) \propto n(t)$ reflects the solution of this rate equation coupled with the sample's thermal relaxation. The characteristic relaxation time τ for the deep-level system is approximately $\tau \sim [e_n + c_n n]^{-1}$. Since e_n is exponentially sensitive to T and P, and n itself changes, the relaxation is non-exponential and depends on the compensation degree K, which sets the Fermi level and equilibrium value of n [4].

Experimental Methods

Samples were prepared from phosphorus-doped silicon by diffusing nickel from a vacuum-deposited layer (99.999% purity) at 1200-1250°C, followed by rapid quenching [5]. This process introduces deep acceptor levels associated with nickel. Control samples (n-Si:P) underwent identical thermal treatment without Ni. The degree of compensation $K = N_{Ni}/N_P$ was varied between 0.1 and 0.9. Specimens (3×3×7

mm³) were equipped with In-Ga eutectic ohmic contacts and a bonded thermocouple. They were mounted in a high-pressure chamber filled with MC transformer oil. Pressure pulses up to $\Delta P = 0.5\ GPa$ were generated with a pneumatic booster, with a rise time $t_r \approx 2-3s$ ($v_p \approx 0.17-0.25 GPa/s$). The sample current I(t) and temperature T(t) were recorded simultaneously with high temporal resolution. Separate isobaric heating experiments were conducted using a miniature heater attached to the sample holder to apply a controlled ΔT at constant pressure.

Results and Discussion

The measured temperature increase of the sample under a $\Delta P = 0.5\ GPa$ pulse was $\Delta T \approx 8-10\ K$ from an initial $T_0 = 295K$, consistent with theoretical estimates for the oil used.

The normalized current $I(t)/I_0$ for a control sample and a compensated n-Si:P,Ni sample with $K \approx 0.8$ was measured. The control sample exhibits a small, prompt increase that saturates with the pressure. The compensated sample displays a complex kinetic: after pressure reaches its maximum at $t = t_0$, the current continues to rise for $\Delta t \approx 3-4\ s$, peaks at I_{max}, and then decays over 5-7 s to a steady-state value I_{st}.

The total relative change can be decomposed as:

$$\mathcal{E}I(t) = \frac{I(t) - I_0}{I_0} = \mathcal{E}_P + \mathcal{E}_{T(t)} + \mathcal{E}_{rel}(t)$$

The static deformational component is $\mathcal{E}_P = (I_{st} - I_0)/I_0$. The transient thermal component is $\mathcal{E}_{T(t)}$, and the kinetic relaxation is $\mathcal{E}_{\mathrm{rel}}(t)$.

Non-Equilibrium Nature of the Transient When the same sample is heated isobarically to achieve the same maximum temperature ΔT_{max}, the current increase is significantly smaller than I_{max} observed during the pressure pulse. This confirms that the transient peak is not a simple thermal effect but involves a **pressure-activated mechanism**. We propose that the combined action of high pressure and elevated temperature during the pulse drives the emission rate e_n(T, P) to a value higher than that achievable at the same temperature but atmospheric pressure, leading to an overshoot in n(t) [2].

Dependence on Compensation Degree and Conductivity Type

The amplitude of the relaxation component, defined as $A_{rel} = (I_{max} - I_{st})/I_{st}$, shows a strong dependence on the compensation degree K for n-type and p-type samples. For K < 0.4, A_{rel} is minimal. As K increases, A_{rel} grows monotonically, and for a given K, it is consistently larger in n-Si:P,Ni than in p-Si:P,Ni. This asymmetry can be explained by the difference in effective mass and deformation potential coupling: light electrons (n-type) couple more strongly to acoustic phonons and lattice vibrations generated by the pressure pulse, enhancing the wave-related relaxation processes implied by the thermal wave model (k-vector).

The observed kinetic sequence of the current response can be interpreted through three consecutive phases. **During the pressure rise ($t < t_0$)**, the primary mechanism is the fast deformational shift of the deep nickel level (the β-effect), which lowers its ionization energy and causes an immediate increase in the free electron concentration n. This process establishes the new steady-state current level I_{st} [5]. **Following pressure stabilization ($t_0 < t < t_max$)**, a thermodeformational overshoot occurs. The sample temperature continues to increase due to heat flow from the adiabatically heated pressure-transmitting fluid. The concurrent action of high pressure P and rising temperature T super-activates the electron emission rate e_n(T, P) from the deep levels, driving the carrier concentration n temporarily above its eventual equilibrium value and resulting in the observed current peak I_{max} [2]. **Subsequently ($t > t_max$)**, the relaxation phase takes place. The sample cools towards the temperature of the pressure cell, while the occupancy of the deep levels re-equilibrates under the condition of constant high pressure. The decay time of the current reflects the combined kinetics of this thermal relaxation and the electronic recombination time constant, which is governed by $\tau \sim [e_n + c_n n]^{-1}$ at the elevated pressure [4].

Conclusion

We have developed a unified model that links thermomechanical wave propagation in the pressure medium with the non-equilibrium kinetics of deep-level ionization in compensated semiconductors under pulsed hydrostatic pressure. The theory introduces a characteristic thermal wavelength $\lambda = 2\pi\sqrt{\chi/(\alpha v_p)}$ dependent on the loading rate. Experiments on n-Si:P,Ni and p-Si:P,Ni reveal a significant kinetic transient in conductivity that exceeds a pure thermal response, demonstrating a pressure-specific enhancement of deep-level emission [2]. The strong dependence of this transient on compensation degree and conductivity type underscores the involvement of carrier-lattice coupling in the relaxation dynamics. These findings are essential for accurately interpreting dynamic pressure experiments and for designing semiconductor sensors intended for pulsed-stress environments.

References:

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