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THE EFFECT OF SAMPLE PRESSURE AND TEMPERATURE ON THE DENSITY OF STATES IN SEMICONDUCTORS

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Abstract
This work explores how hydrostatic (all-round) pressure and temperature modify the band structure and the density of states in n-Si⟨Ni⟩ and n-Si⟨Co⟩ samples. Experimental evidence indicates that pressure-driven breakup of nickel- and cobalt-related impurity clusters generates additional localized levels within the band gap and causes a pronounced, multi-fold rise in the resistivity. Incorporating temperature effects on the band-gap width, the carrier effective mass, and the Fermi–Dirac distribution, we propose a theoretical framework describing the density of states g(E,P,T), the free-carrier concentration n(P,T), and the resistivity ρ(P,T) in terms of the deformation (pressure) energy E_def(P) and temperature T. The combined impact of pressure and temperature is discussed qualitatively, demonstrating that increasing temperature progressively smooths the step-like features observed in the ρ/ρ₀(P) dependence.

Keywords: Pressure energy; temperature; semiconductor; density of states; impurity cluster; nickel; cobalt.

Introduction

In semiconductors, changes in external pressure and temperature modify the energy bands and the density of states (DOS), which in turn leads to a controllable change in electrical conductivity [1–3]. Under hydrostatic (all-round) pressure (HTGB), the volumetric deformation of the crystal lattice significantly affects the band-gap width E_g, valley splitting, the effective mass m*, and the stability of impurity clusters.

Turgunov and co-authors [1] studied the HTGB effect in n-Si⟨Ni⟩ and n-Si⟨Co⟩ single-crystal samples

in the pressure range P = 10^8–1.6·10^9 Pa. Their work reported a sharp, two-step increase of the normalized resistivity ρ/ρ0(P) as pressure rises. Electron microprobe analysis showed that clusters decay under pressure in a certain sequence, and that the corresponding processes depend on the clusters' size and shape.

In the present paper, these experimental results are theoretically generalized, and the influence of pressure energy E_def(P) and temperature T on the density of states g(E,P,T) and on transport properties is analyzed.

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Brief analysis of experimental data

For n-Si⟨Ni⟩ and n-Si⟨Co⟩ samples, the ρ/ρ0(P) curve reported in [1] has the following features (at temperatures around 300 K): for the initial n-Si sample, ρ/ρ0(P) ≈ 1, i.e., the pressure effect is small; for n-Si⟨Ni⟩ samples, the first step is observed at P ≈ 6·10^8 Pa and the second at P ≈ 1.2·10^9 Pa, with an overall increase up to ~10 times; for n-Si⟨Co⟩ samples, steps appear near P ≈ 4·10^8 Pa and 8·10^8 Pa, and ρ/ρ0 increases up to ~13 times.

According to electron microprobe analysis, the first step corresponds to the decay of small needle-like and disk-like clusters, whereas the second step corresponds to the decay of comparatively larger lens-shaped and spherical clusters. This indicates a sharp pressure-induced increase of the density of deep localized levels N_t(P) inside the forbidden gap.

Theoretical model of pressure energy and temperature

Pressure energy and band-edge shifts. Under HTGB, the relative change of the crystal volume V is

$$\frac{\Delta V}{V} \approx -\frac{P}{B} \qquad (1)$$

where B is the bulk modulus of silicon (~10^11 Pa). The corresponding elastic energy density (pressure energy) is

$$E_{\text{def}}(P) \approx \frac{1}{2} B \left(\frac{\Delta V}{V}\right)^2 \approx \frac{P^2}{2B} \qquad (2)$$

Using the deformation potentials a_c and a_v, the pressure dependence of the conduction- and valence-band edges can be written as:

$$E_c(P) = E_c(0) + a_c \frac{\Delta V}{V}, \qquad E_v(P) = E_v(0) + a_v \frac{\Delta V}{V} \qquad (3)$$

As a result, under pressure the band-gap width is

$$E_g(P) = E_c(P) - E_v(P) \qquad (4)$$

and the conduction-band density of states g_c(E,P) changes accordingly.

Effect of temperature on the band gap and DOS. The temperature dependence of the band gap is often described by the Varshni relation:

$$E_g(T) = E_g(0) - \frac{\alpha T^2}{T + \beta} \qquad (5)$$

where α and β are empirical parameters [2]. Accordingly,

$$E_c(P,T) = E_c(P,0) - \frac{1}{2}\Delta E_g(T), \qquad E_v(P,T) = E_v(P,0) + \frac{1}{2}\Delta E_g(T), \quad (6)$$

i.e., pressure deforms (typically widens/shifts) the gap, while temperature tends to narrow it. For a parabolic spectrum, the conduction-band DOS is:

$$g_c(E,P,T) = \frac{1}{2\pi^2}\left(\frac{2m_c^*(P,T)}{\hbar^2}\right)^{3/2} \sqrt{E - E_c(P,T)}, \qquad E \geq E_c(P,T), \quad (7)$$

and the integrated effective density of states is

$$N_c(P,T) = 2\left(\frac{2\pi m_c^*(P,T) kT}{h^2}\right)^{3/2} \propto T^{3/2} \qquad (8)$$

Thus, as temperature increases, the number of "active" states in the conduction band increases.

Impurity clusters and trap-state density. Under pressure, the decay of nickel and cobalt clusters leads to the appearance of deep local levels inside the forbidden gap [1]. In a simplified model, the total trap density is described as

$$N_t(P) = \begin{cases} N_{t0}, & P < P_1, \\ N_{t0} + \Delta N_{t1}, & P_1 \le P < P_2, \\ N_{t0} + \Delta N_{t1} + \Delta N_{t2}, & P \ge P_2, \end{cases} \quad (9)$$

in the form shown above.

If the energy of a trap level is E_{t,i}(P), its occupancy is given by the Fermi–Dirac distribution:

$$f_{t,i}(P,T) = \frac{1}{1 + g_i \exp\left(\frac{E_{t,i}(P) - E_F(P,T)}{kT}\right)} \quad (10)$$

where g_i is the degeneracy factor. The density of ionized centers that capture electrons is:

$$N_t^-(P,T) = \sum_i N_{t,i}(P)\, f_{t,i}(P,T) \quad (11)$$

Charge neutrality and free-carrier concentration. For an n-type semiconductor, the charge neutrality condition is:

$$n(P,T) + N_A^-(P,T) + N_t^-(P,T) \approx N_D^+(P,T) \quad (12)$$

If there is no strong degeneracy, the free-electron concentration is

$$n(P,T) \approx N_c(P,T) \exp\left[-\frac{E_c(P,T) - E_F(P,T)}{kT}\right] \quad (13)$$

The density of "active" states participating in transport is

$$g_{\text{eff}}(P,T) = \int g(E,P) \left[-\frac{\partial f(E, E_F, T)}{\partial E}\right] dE, \quad (14)$$

where f is the Fermi–Dirac function. The quantity $-\partial f/\partial E$ represents an energy window of width ~4kT around the Fermi level; as temperature increases this window broadens and "activates" a much larger portion of g(E,P).

Pressure- and temperature-dependence of the resistivity

Electrical conductivity and resistivity:

$$\sigma(P,T) = \frac{1}{\rho(P,T)} = q\,\mu(P,T)\,n(P,T) \quad (15)$$

$$\rho(P,T) = \frac{1}{q\,\mu(P,T)\,n(P,T)} \quad (16)$$

Here μ(P,T) is the mobility, which decreases approximately as μ ∝ T^{−m} (m ≈ 1.5) due to phonon scattering; under HTGB it may also vary because of lattice defects and cluster decay.

Results and discussion

Based on the theoretical expressions, the influence of pressure and temperature on free carriers and on the DOS can be analyzed in three temperature ranges. Low temperatures (cryogenic regime): when kT ≪ |E_{t,i} − E_F|, traps are almost fully occupied or empty and thermal emission is very weak. In an n-type sample, donors are also not fully ionized, so n(P,T) is small. Pressure energy may break up clusters, but because the number of carriers participating in transport is small, ρ(P,T) is very large for any P and the steps in ρ/ρ0(P) are not pronounced.

Intermediate temperatures (around 300 K): the experiments in [1] were performed in this regime. At this temperature donors are mostly ionized, while trap levels are located near the Fermi level so that 0 < f_{t,i} < 1. Therefore, at P1 and
P2, a sharp increase of N_t(P) leads to a sharp increase of N_t^−(P,T) and to a several-fold decrease of n(P,T). As a result, the two-step rise of ρ/ρ0(P) is observed most clearly.
High temperatures (T ≳ 450 K): as temperature increases, N_c(P,T) ∝ T^{3/2} grows, thermal emission from traps becomes stronger, and electrons can more readily escape from deep levels into the conduction band. On the one hand μ(T) decreases due to phonon scattering; on the other hand n(P,T) increases noticeably. Hence the overall value of ρ(P,T) may not be large, and the step-like features caused by pressure become smoothed: ρ/ρ0(P) remains pressure-dependent but forms a smooth curve instead of sharp steps.
To facilitate understanding of this behavior, Figure 1 shows a model ρ/ρ0(P) curve for different temperatures.

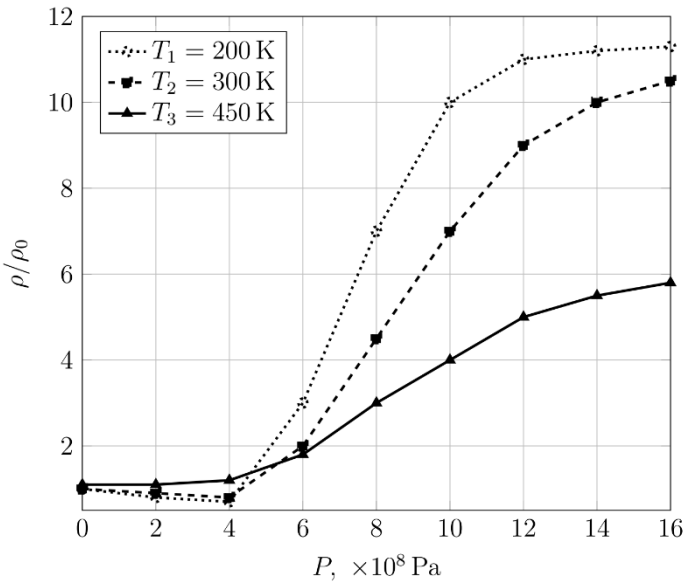

Figure 1. Model dependence of the normalized resistivity on pressure and temperature.

At low temperatures (T1) the steps in ρ/ρ0(P) are very sharp; at intermediate temperature (T2 ≃ 300 K) a two-step behavior matching the experiment appears; at high temperature (T3) the steps are smoothed due to thermal emission.
Trap density and free-carrier concentration. Under HTGB, the trap density N_t(P) is mainly determined by pressure and increases sharply near P1 and P2 (cluster decay). However, the free-carrier concentration n(P,T) is controlled by both pressure and temperature. Figure 2 presents a relative model dependence of N_t(P) and n(P,T). As can be seen from Figure 2, at low temperatures traps “hold” electrons strongly and n(P,T1) remains very small, while at intermediate temperature
(T2) a noticeable drop of n(P,T) near P1 and P2 corresponds to the steps in ρ/ρ0(P). At high temperatures (T3), even though N_t(P) is large, n(P,T3) stays at higher values because thermal emission from traps is enhanced, and it varies more smoothly with pressure.

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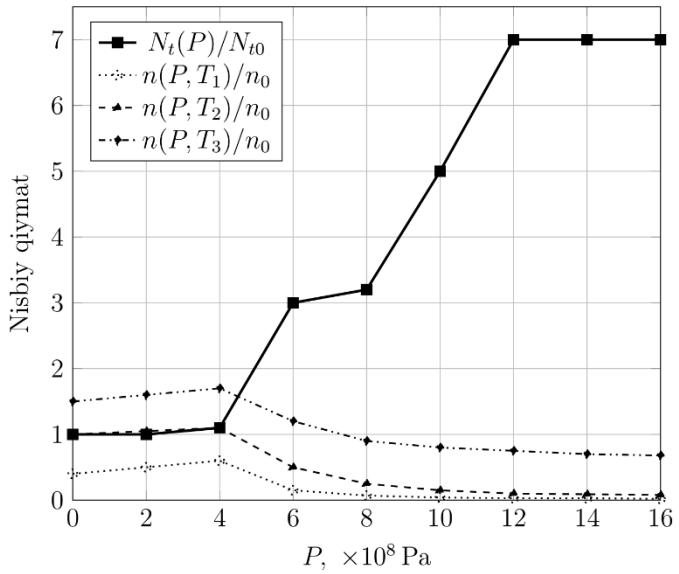

Figure 2. Model pressure- and temperature-dependence of the trap-state density N_t(P) and the relative free-electron concentration n(P,T).

As pressure increases, cluster decay raises N_t(P) step-by-step, and at low and intermediate temperatures n(P,T) decreases sharply. At high temperatures, stronger thermal emission makes n(P,T) less sensitive to pressure.

Temperature dependence of the DOS at high pressure. To illustrate the energy distribution of trap states and how their influence weakens with increasing temperature, Figure 3 schematically compares the DOS at high pressure (P > P2) for low and high temperatures.

At low T, local peaks in g(E) strongly affect transport, and trap levels play a major role in capture and scattering processes. At high T, the broader Fermi window around E_F causes averaging over a wider DOS region, so the sharp steps in ρ/ρ0(P) are gradually washed out.

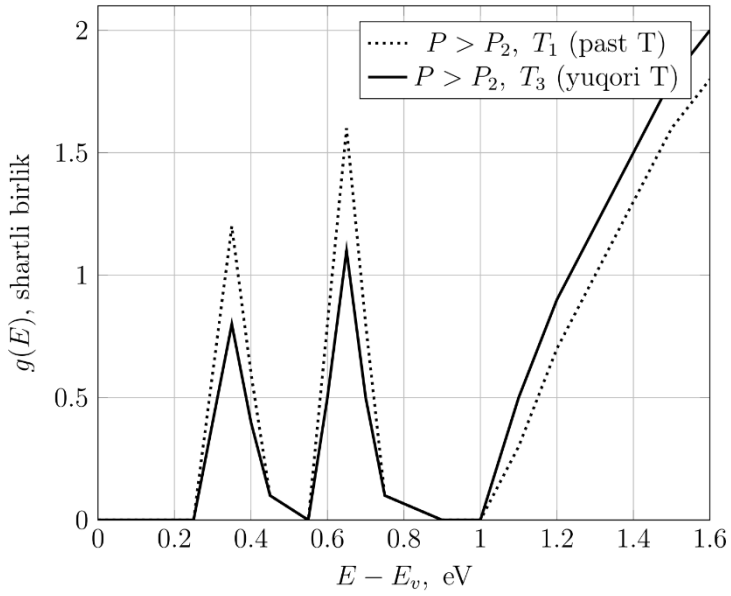

Figure 3. Schematic comparison of the DOS at high pressure (P > P2) for low and high temperatures.

Trap peaks are clearly visible near E_{t,i}, while above the conduction-band edge g_c(E) increases. As temperature rises, the Fermi–Dirac window broadens, so the trap peaks appear "washed out" from the transport viewpoint.

Pressure energy–temperature–DOS triangle. The interrelation between pressure energy E_def(P), temperature T, and the density of states g(E,P,T) can be summarized as follows:

Pressure energy deforms the crystal lattice and breaks up impurity clusters: E_c(P,T) and E_v(P,T) shift, E_g(P) changes, and N_t(P) increases sharply near P1 and P2.

Temperature reduces the band gap, increases N_c(P,T), and broadens the Fermi–Dirac window; consequently, a much larger part of g(E,P) contributes to transport. At low T, the structural effect of pressure is not fully manifested in transport; at intermediate T the steps in ρ/ρ0(P) are the most pronounced; at high T the steps are smoothed due to thermal emission.

Conclusion

In n-Si⟨Ni⟩ and n-Si⟨Co⟩ samples, the decay of impurity clusters under HTGB leads to the formation of deep local levels within the forbidden gap, i.e., to a significant redistribution of the density of states. As pressure energy E_def(P) increases, N_t(P) grows step-by-step and produces a two-step rise of the normalized resistivity ρ/ρ0(P) at intermediate temperatures. Temperature, through its influence on the band gap, effective mass, and Fermi–Dirac statistics, controls the effective density of states in the conduction band N_c(P,T) and the trap occupancy N_t^−(P,T), as well as the free-carrier concentration n(P,T). The theoretical analysis and the model plots in Figures 1–3 indicate that the joint action of pressure energy and temperature smooths the pressure dependence of ρ(P,T) at low and high temperatures, whereas the steps in ρ/ρ0(P) are most clearly expressed in the intermediate temperature range.

The proposed g(E,P,T) and ρ(P,T) model can serve as a theoretical basis for pressure and temperature sensors based on n-Si⟨Ni⟩ and n-Si⟨Co⟩, as well as for optimizing the density of states when designing cluster-containing semiconductor structures.

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