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DENSITY OF STATES OF N-SI⟨NI⟩ AND N-SI⟨CO⟩ UNDER PRESSURE VARIATIONS APPLIED TO THE SAMPLE

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Abstract

This study examines the influence of uniform hydrostatic pressure (UHP) on the relative resistivity $\rho/\rho_0(P)$ of n-Si⟨Ni⟩ and n-Si⟨Co⟩ single-crystal samples and, on this basis, analyzes how the semiconductor density of states g(E,P) depends on the pressure- (deformation-) related energy. As pressure increases, the step-by-step disintegration of neutral nickel and cobalt impurity clusters results in a pronounced rise in the number of deep localized levels $N_t(P)$ within the band gap, a reduction in the free-electron concentration n(P), and a two-stage increase in $\rho/\rho_0(P)$. Using the experimental observations, qualitative links among the deformation energy E_def(P), the localized-state density $N_t(P)$, and the resistivity $\rho(P)$ are discussed, and representative plots of $\rho/\rho_0(P)$, $N_t(P)$, and g(E,P) are presented for three characteristic pressure regimes.

Keywords: hydrostatic pressure; pressure energy; semiconductor; density of states; impurity cluster; localized levels; nickel; cobalt.

Introduction

The influence of external pressure on semiconductors is an important tool for controlling their band structure and electrical properties. Under uniform hydrostatic pressure (UHP), the volumetric deformation of the crystal lattice changes the band-gap width E_g(P), the splitting of valleys, and the effective mass m*(P), and it also has a substantial effect on the stability of impurity clusters [1,2].

As a result of diffusion of 3d elements (Ni, Co) into n-type Si, electrically neutral impurity clusters are formed inside the crystal. In the works of Turgunov and co-authors [3], the resistivity of n-Si⟨Ni⟩ and n-Si⟨Co⟩ samples was measured under UHP in the range $P = 10^8–1.6\cdot10^9$ Pa, and a two-step increase of $\rho/\rho_0(P)$ was revealed. Morphological analysis shows that these steps correspond to the breakup of small needle-like/disk-like clusters and large lens-like/spherical clusters, respectively.

The aim of this work is to qualitatively analyze, on the basis of these experimental results, how the density of states g(E,P) and the density of localized states $N_t(P)$ are redistributed as the pressure energy E_def(P) changes, and to relate this redistribution to the $\rho/\rho_0(P)$ curve.

Object of study and measurements under UHP

The objects of study were n-Si⟨Ni⟩ and n-Si⟨Co⟩ samples prepared on the basis of KEF-grade single-crystal n-type silicon [3]. Diffusion of Ni and Co was carried out for several hours at about ~1523 K, resulting in the formation of impurity clusters of different sizes and shapes in the bulk of the samples. Such electrically neutral clusters can be needle-like, disk-like, lens-like, or spherical, with sizes ranging from hundreds of nanometers to several micrometers.

UHP was applied to the samples using a special LG-16-type apparatus in the range $P = 10^8–1.6\cdot10^9$ Pa. Measurements were performed at nearly constant (room) temperature. At each pressure value, the resistivity ρ(P) was measured, and the curve $\rho/\rho_0(P)$ was constructed relative to the zero-pressure value ρ_0.

In accordance with the experimental results, a schematic model of $\rho/\rho_0(P)$ is shown in Fig. 1.

As can be seen from Fig. 1, for n-Si the effect of pressure is almost unnoticeable: elastic deformation of the crystal lattice only weakly changes the band structure, and $\rho/\rho_0(P) \simeq 1$. In n-Si⟨Ni⟩ and n-Si⟨Co⟩ samples, however, a two-stage increase is observed with increasing pressure: the first step ($P \approx P_1$) corresponds to the breakup of small needle-like/disk-like clusters, whereas the second step ($P \approx P_2$) corresponds to the breakup of large lens-like/spherical clusters.

Pressure energy and band-edge shifts

Under hydrostatic pressure, the crystal volume V changes approximately as:

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

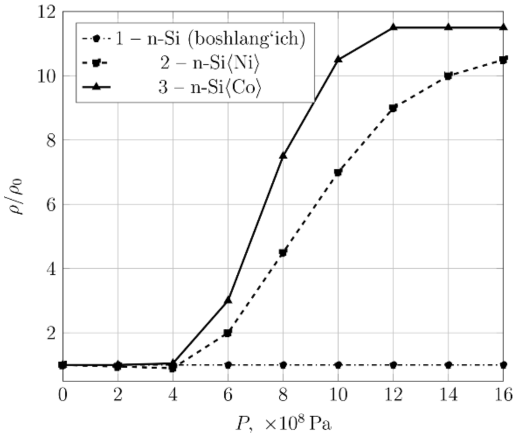

Figure 1. Relative resistivity versus pressure for n-Si, n-Si⟨Ni⟩, and n-Si⟨Co⟩ samples (schematic model).

For the initial n-Si, $\rho/\rho_0(P) \approx 1$. For the doped samples, a two-step increase of $\rho/\rho_0(P)$ is observed around P_1 and P_2 due to the breakup of impurity clusters.

The elastic energy density associated with volumetric deformation (pressure energy) can be written as:

$$E_{\text{def}}(P) \approx \frac{P^2}{2B} \qquad (2)$$

where B is the bulk modulus (for silicon, of order $\sim 10^{11}$ Pa).

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, the band-gap width is

E_g(P) = E_c(P) − E_v(P). (4)

Consequently, the density of states in the conduction band g_c(E,P) changes with pressure.

For a conduction band with a parabolic spectrum, the density of states is:

$$g_c(E,P) = \frac{1}{2\pi^2}\left(\frac{2m_c^*(P)}{\hbar^2}\right)^{3/2}\sqrt{E - E_c(P)} \qquad (5)$$

Here m_c*(P) is the pressure-dependent effective mass. At low pressures ($P < P_1$), valley splitting and changes in lattice parameters can reduce E_c(P) and slightly increase g_c(E_F,P). Therefore, the density of states near the Fermi level increases and the concentration of free carriers n(P) in the conduction band increases. This corresponds to an initial decrease in ρ(P) (Fig. 1).

Impurity clusters and the density of localized states $N_t(P)$

Clusters formed as a result of diffusion of Ni and Co atoms are, under zero pressure, mostly electrically neutral and therefore do not play a significant role in charge transport. Under UHP, when E_def(P) becomes comparable to the binding energy of clusters, they start to break up—first the small clusters and then the large ones. In a simplified model, we represent the density of localized states in the band gap by three regions:

$$N_t(P) = \begin{cases} N_{t0}, & P < P_1, \\ N_{t0} + \Delta N_{t1}, & P_1 \le P < P_2, \\ N_{t0} + \Delta N_{t1} + \Delta N_{t2}, & P \ge P_2. \end{cases} \qquad (6)$$

A schematic plot of this function is shown in Fig. 2.

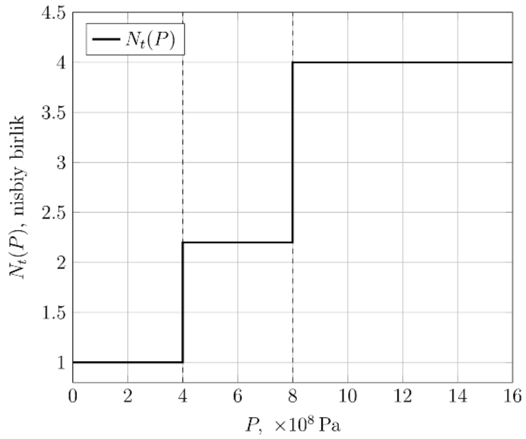

Figure 2. Schematic dependence of the density of localized states $N_t(P)$ on pressure (relative units).

Thus, Figs. 1 and 2 together indicate the following sequence:

- Elastic deformation stage ($P < P_1$): small shifts of the band edges, an increase in g_c(E_F,P), a slight decrease of $\rho/\rho_0(P)$, and $N_t(P) \approx N_t0$.
- Breakup of small clusters ($P_1 \leq P < P_2$): the first sharp increase of $N_t(P)$; due to the growth of localized states the number of free carriers decreases, and $\rho/\rho_0(P)$ rises sharply as the first step.
- Breakup of large clusters ($P \geq P_2$): the second sharp increase of $N_t(P)$, a reduction of the share of extended (free) states, and the second step of $\rho/\rho_0(P)$.

For $P < P_1$ the clusters remain mostly intact and the number of localized states is N_t0. At $P \approx P_1$, breakup of small needle-like and disk-like clusters causes the localized-state density to jump to $N_t0 + \Delta N_t1$. At $P \approx P_2$, breakup of large lens-like and spherical clusters produces a second sharp increase of $N_t(P)$.

Redistribution of the density of states g(E,P)

The three stages above can be illustrated more clearly using density-of-states diagrams. Figure 3 shows schematic plots of g(E,P) for three pressure regimes:

- $P < P_1$: only a small number of localized states close to the band edges; g_t(E,P) is small.
- $P_1 \leq P < P_2$: the density of localized states increases and g_t(E,P) noticeably "fills" the band gap.
- $P \geq P_2$: deep states become very abundant and the fraction of extended (free) states decreases.

The three curves in Fig. 3 can be interpreted briefly as follows:

- $P < P_1$ (elastic deformation): g_c(E,P) increases slightly, while g_t(E,P) remains as a small additional "tail".
- $P_1 < P < P_2$ (breakup of small clusters): new deep levels appear in the band gap, g_t(E,P) occupies a significant part of it, which corresponds to the first step of $\rho/\rho_0(P)$.
- $P \geq P_2$ (breakup of large clusters): the density of deep states is maximal, the share of free states decreases, and $\rho/\rho_0(P)$ reaches the second step.

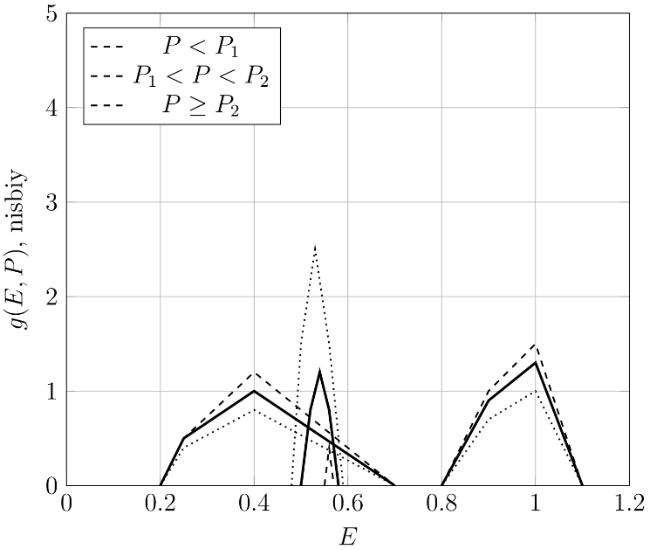

Figure 3. Schematic plots of the density of states g(E,P) in three pressure regimes. With increasing pressure, (a) the conduction-band edge E_c(P) shifts and the density of extended states g_c(E,P) changes slightly, while (b) the density of localized states g_t(E,P) inside the band gap increases sharply. For $P < P_1$, localized states are scarce; for $P_1 < P < P_2$, deep localized states grow; for $P \geq P_2$, localized states dominate and the fraction of extended states decreases.

Conclusion

Experimental results obtained from resistivity measurements of n-Si⟨Ni⟩ and n-Si⟨Co⟩ samples under UHP show a pronounced redistribution of the density of states in the semiconductor as the pressure energy changes. While the pressure effect in the initial n-Si is almost negligible (Fig. 1, curve 1), in n-Si⟨Ni⟩ and n-Si⟨Co⟩ doped with 3d elements the step-by-step breakup of impurity clusters causes a sharp increase in the number of deep localized levels $N_t(P)$ in the band gap (Fig. 2), a redistribution of g(E,P) (Fig. 3), and a two-step rise of $\rho/\rho_0(P)$ (Fig. 1). Accordingly, three stages can be clearly distinguished: (i) elastic deformation—band-edge shifts and an increase of g_c(E_F,P); (ii) breakup of small clusters—the first sharp increase of g_t(E,P) and the first step of $\rho/\rho_0(P)$; (iii) breakup of large clusters—the second sharp increase of g_t(E,P), a decrease in the share of free states, and the second step of $\rho/\rho_0(P)$.

The proposed simple model

$g(E,P) = g_c(E,P) + g_t(E,P)$. (7)
describes the pressure-dependent density of states and qualitatively agrees well with the experimental $\rho/\rho_0(P)$ curve. It may serve as a theoretical basis for designing high-pressure sensors and cluster-containing semiconductor structures based on n-Si⟨Ni⟩ and n-Si⟨Co⟩.

References

1. C. Kittel, Introduction to Solid State Physics, 8th ed. (John Wiley & Sons, 2005).
2. S. M. Sze, K. K. Ng, Physics of Semiconductor Devices, 3rd ed. (John Wiley & Sons, 2007).
3. N. A. Turgunov, E. Kh. Berkinov, D. Kh. Mamajonova, “Decay of impurity clusters of nickel and cobalt atoms in silicon under the influence of pressure”, Journal of Nano- and Electronic Physics, 13(5), 05006 (2021).