

# STRUCTURE AND CHEMICAL COMPOSITION OF MICRO- AND NANO-INCLUSIONS OF NI IN SILICON

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**Abstract** This paper presents a study of the morphology, structure, and chemical composition of nickel (Ni) micro- and nano-inclusions formed in silicon after diffusion annealing under different cooling rates. The investigation was carried out using electron probe microanalysis (EPMA) on a Superprobe JXA-8800R system. The results demonstrate that the size, density, and geometric shape of Ni-related inclusions strongly depend on the cooling rate after diffusion annealing. Rapid cooling ( $v_c = 600$  °C/s) leads to the formation of small, thermodynamically non-equilibrium inclusions with needle-like, disk-like, plate-like, and lens-shaped morphologies. Slow cooling ( $v_c < 1$  °C/s) promotes the growth of larger, predominantly spherical and multilayer inclusions. The structural differences between n-type and p-type Si<Ni> samples are analyzed. It is shown that inclusion morphology evolves from anisotropic forms at small sizes to spherical shapes as the size increases. The findings provide insight into the precipitation mechanisms of nickel silicides in silicon and their dependence on thermal treatment conditions.

**Keywords:** silicon, nickel, microinclusions, nanoinclusions, diffusion annealing, cooling rate, nickel silicides, precipitation, EPMA.

## INTRODUCTION

Nickel is one of the most technologically significant metal impurities in silicon. Due to its high diffusivity and strong interaction with intrinsic defects, Ni can form various structural defects and precipitates in silicon during high-temperature treatments. These precipitates significantly influence the electrical and structural properties of silicon, affecting carrier lifetime, recombination processes, and mechanical stability.

Understanding the formation mechanisms, morphology, and structure of nickel-related micro- and nano-inclusions is essential for both fundamental semiconductor physics and applied silicon technology. The precipitation process is highly sensitive to thermal conditions, especially the cooling rate after diffusion annealing.

This study investigates the structure and chemical composition of Ni microinclusions formed in n-type and p-type silicon under different cooling regimes.

## **EXPERIMENTAL METHOD**

The morphology and chemical composition of nickel-related microinclusions were studied using electron probe microanalysis (EPMA) with a Superprobe JXA-8800R system.

Silicon samples doped with nickel (Si<Ni>) were subjected to diffusion annealing followed by controlled cooling under two regimes:

Rapid cooling:  $v_c = 600$  °C/s to Slow cooling:  $v_c < 1$  °C/s

Both n-type (n-Si<Ni>) and p-type (p-Si<Ni>) samples were analyzed.

Microstructural observations were performed to determine:

Inclusion size, Geometric shape, Density distribution and Layered structure

Chemical composition (nickel silicides)

## **RESULTS AND DISCUSSION**

**Microinclusions in n-Si<Ni> with Rapid Cooling ( $v_c = 600$  °C/s)**

In n-type silicon rapidly cooled after diffusion annealing, microinclusions with sizes up to  $\sim 10^{-6}$  m were observed.

The inclusions exhibited the following morphologies:

Needle-like, Disk-like and Lens-shaped

Electron probe analysis showed that these inclusions consist of one or several layers of nickel silicides. Their average density was approximately:  $\sim 2 \times 10^3 \text{ cm}^{-3}$

The relatively small size and anisotropic shapes indicate that rapid cooling suppresses diffusion-driven coarsening and stabilizes thermodynamically non-equilibrium structures

#### **Microinclusions in n-Si<Ni> with Slow Cooling ( $v_c < 1 \text{ }^\circ\text{C/s}$ )**

In slowly cooled n-Si<Ni> samples, significantly larger microinclusions were formed, with sizes reaching up to  $\sim 10^{-5}$  m.

Their characteristics include: Lens-shaped forms, Spherical shapes and Polyhedral shapes close to spherical, These inclusions exhibit a multilayer structure, indicating sequential precipitation of different nickel silicide phases.

The average density was:  $\sim 5 \times 10^2 \text{ cm}^{-3}$

The lower density but larger size suggests coalescence and growth processes during prolonged cooling.

#### **Microinclusions in p-Si<Ni> with Rapid Cooling**

In p-type silicon rapidly cooled at  $600 \text{ }^\circ\text{C/s}$ , microinclusions of various shapes were observed: Needle-like, Disk-like, Lens-shaped and Spherical

Their sizes reached up to:  $3 \times 10^{-7}$  m to The density was approximately:  $\sim 10^3 \text{ cm}^{-3}$

Unlike n-type samples, these inclusions were predominantly monolayer structures composed of a single nickel silicide phase.

#### **Microinclusions in p-Si<Ni> with Slow Cooling**

In p-Si<Ni> samples cooled at  $v_c < 1$  °C/s, inclusions of multiple shapes formed, with larger ones being predominantly spherical.

Maximum size:  $3 \times 10^{-6}$  m and Density:  $\sim 10^2$  cm<sup>-3</sup>. Most inclusions exhibited multilayer structures.

### **Influence of Cooling Rate on Inclusion Morphology**

The experimental results clearly demonstrate that the geometry and size distribution of Ni microinclusions are strongly dependent on the cooling rate after diffusion annealing.

Higher cooling rate → smaller inclusions, Higher cooling rate → anisotropic, non-equilibrium shapes, Lower cooling rate → larger, spherical inclusions and Lower cooling rate → multilayer structure levels

Small inclusions tend to have needle-like, disk-like, plate-like, and lens-shaped morphologies. As their size increases, the shape becomes predominantly spherical due to surface energy minimization.

Rapid cooling increases the probability of forming thermodynamically non-equilibrium inclusions with irregular geometry. Slow cooling allows sufficient time for diffusion-driven growth and structural ordering.

### **Mechanism of Nickel Silicide Formation**

Nickel has high diffusivity in silicon, which enables rapid migration during annealing. Upon cooling: Supersaturation of Ni occurs, Nucleation of nickel silicide phases begins, Growth depends on diffusion kinetics and Coalescence may occur at low cooling rates condition

The multilayer structure suggests phase transitions or sequential precipitation of different silicide phases during temperature decrease.

## **CONCLUSION**

Based on the experimental investigations of Ni micro- and nano-inclusions in silicon, the following conclusions can be drawn:

1. The size, density, and morphology of nickel-related inclusions strongly depend on the cooling rate after diffusion annealing.

2. Rapid cooling (600 °C/s) leads to the formation of small ( $\sim 10^{-6}$ – $10^{-7}$  m), anisotropic, thermodynamically non-equilibrium inclusions with needle-like, disk-like, and lens-shaped morphologies.

3. Slow cooling ( $< 1$  °C/s) promotes the formation of larger ( $\sim 10^{-5}$ – $10^{-6}$  m), predominantly spherical inclusions with multilayer structure.

4. Inclusion density decreases as cooling rate decreases, while average size increases.

5. The morphology evolution from anisotropic to spherical shapes is governed by diffusion processes and surface energy minimization.

6. Differences between n-Si<Ni> and p-Si<Ni> samples indicate that conductivity type influences precipitation behavior and structural characteristics of nickel silicides.

The obtained results contribute to understanding precipitation mechanisms of transition metal impurities in silicon and can be used for optimization of thermal processing in semiconductor technology.

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