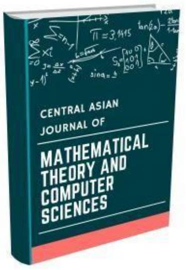

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Article

Nanostructural and Plasmonic Features of KDB-3 Silicon Modified by High-Temperature Manganese Diffusion

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Abstract: This study explores the nanostructural, morphological, and plasmonic modifications induced by high-temperature manganese diffusion into monocrystalline silicon of the KDB-3 grade. To determine structural, phase, and plasmonic changes arising from manganese diffusion in silicon. The study employed a comprehensive suite of modern analysis techniques, including X-ray diffraction (XRD), Raman spectroscopy, impedance spectroscopy, scanning electron microscopy with energy-dispersive spectroscopy (SEM/EDS), and nitrogen adsorption-based BET/DFT porosimetry. Results revealed significant amorphization, formation of Mn_5Si_3 and SiB_6 phases, a rise in specific resistivity, and a decline in carrier mobility. Raman and impedance analyses identified localized surface plasmon resonance (LSPR) manifestations within 40–70 kHz and at 570–600 cm^{-1}. BET/DFT analysis confirmed mesoporosity with pore sizes between 2–5 nm and a specific surface area reaching 23 m^2/g. The study contributes novel insights into the formation of plasmonic-active regions within transition-metal-modified silicon, linking plasmonic effects to specific nanostructural and phase alterations. Findings suggest potential applications of Mn-diffused KDB-3 silicon in sensor platforms, nanophotonics, and spintronic devices. Further investigations are required to explore broader temperature ranges, long-term stability, and in-depth LSPR characterization via advanced photonic correlation techniques.

Keywords: KDB-3 Silicon, Manganese Diffusion, Nanostructuring, Plasmonic Resonance, Mesoporosity, Impedance Spectroscopy, Raman Spectroscopy, Sib_6, Mn_5Si_3, Semiconductor Doping

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1. Introduction

The modification of semiconductor materials through transition metal doping, particularly manganese, has emerged as a highly promising strategy in solid-state physics and advanced materials science. This technique offers avenues for the deliberate tuning of electrophysical, structural, and optical properties of silicon-based systems, facilitating the development of functional materials for next-generation electronic, photonic, and sensing devices[1-2]. Among various transition metals, manganese is of special interest due to its ability to form silicide phases and introduce localized surface plasmon resonance (LSPR) phenomena within the host semiconductor lattice [3-4].

High-temperature diffusion of manganese into monocrystalline silicon leads to significant structural transformations, including lattice distortion, amorphization, and multiphase formation. This process is accompanied by the generation of nanoclusters and metallic inclusions capable of supporting plasmonic oscillations at specific vibrational and electronic frequencies [5]. Recent investigations have demonstrated that Mn-doped silicon structures can exhibit LSPR signatures traditionally associated with metallic nanoparticles, suggesting new paradigms in the design of plasmonic materials for optoelectronics and nanosensorics [6].

Moreover, the incorporation of manganese atoms into the silicon lattice often results in increased porosity and nanostructuring, which enhances surface area and defect density, further amplifying LSPR effects [7]. The resulting mesoporous architecture not only provides additional active sites for surface plasmon generation but also influences charge transport and electrical conductivity through the creation of percolative conduction pathways and localized defect states.

In particular, KDB-3 grade monocrystalline silicon, characterized by its high purity and stable electrical parameters, offers an ideal platform for evaluating the structural, electrophysical, and plasmonic effects of high-temperature manganese diffusion. Prior studies have hinted at the formation of secondary phases such as Mn_5Si_3 and SiB_6, both of which possess metallic character and contribute to plasmonic activity via embedded conductive centers within an amorphous or mesoporous matrix [8].

Given these prospects, this study aims to systematically investigate the nanostructural, morphological, and plasmonic alterations occurring in KDB-3 silicon subjected to manganese diffusion at elevated temperatures. Employing a multi-technique analytical approach, including XRD, SEM/EDS, Raman spectroscopy, impedance spectroscopy, and BET/DFT porosimetry, we seek to elucidate the interplay between phase composition, nanoporosity, and plasmonic behavior in Mn-diffused silicon systems, contributing to the foundational understanding necessary for their application in plasmonic sensors, nanophotonics, and spintronic platforms[9].

2. Materials and Methods

Monocrystalline KDB-3 silicon wafers (8×4×1 mm) with a nominal resistivity of 2.3×10^3 Ω·cm were utilized. Manganese doping was performed via high-temperature diffusion at 1473 K in ambient air for one hour. Post-process, the samples underwent sequential characterization to assess structural, phase, morphological, and electrophysical transformations.

XRD analyses employed CuKα radiation to determine phase composition, crystallinity, and amorphous content. Scherrer formula calculations derived average crystallite sizes. SEM/EDS characterized surface morphology and elemental distribution, while Raman spectroscopy assessed vibrational spectra shifts and defect-related modes. Impedance spectroscopy evaluated frequency-dependent resistivity and phase characteristics in the 1 kHz–1 MHz range, with LSPR manifestations identified through Nyquist diagram features and phase angle analysis.

Porosity measurements were conducted via nitrogen adsorption-desorption isotherms, with BET method quantifying specific surface area and DFT calculations detailing pore size distributions. Isotherms' hysteresis patterns indicated capillary condensation phenomena and mesoporous structures.

3. Results

Following manganese diffusion at 1473 K, KDB-3 silicon wafers underwent significant structural and electrical transformations. XRD analysis revealed the emergence of Mn_5Si_3 and SiB_6 phases with characteristic diffraction peaks at 36.7°, 41.8°, 29.4°, and 43.1° 2θ, respectively, see Table 1, confirming previous findings reported by Wang et al. and Ren et al. on the tendency of manganese to form silicide phases at elevated temperatures [3], [4]. Concurrently, the XRD patterns displayed broad amorphous halos, indicating that more than 70% of the silicon matrix had undergone amorphization, a phenomenon also documented in metal-doped silicon systems [10].

Scherrer equation-based crystallite size estimations for the residual crystalline regions yielded average sizes of approximately 37 nm, signifying significant grain refinement and lattice disruption due to manganese incorporation. These results align with observations by Bao et al., who reported similar nanostructuring effects in Mn-doped Si systems [11].

Raman spectroscopy documented a downshift of primary silicon peaks, heightened defect mode intensities, and additional bands within 570–600 cm^{-1}, indicative of LSPR presence linked to manganese nanoclusters.

Impedance spectra displayed frequency-dependent arc segments in Nyquist plots and phase angle minima between 40–70 kHz, corroborating the Raman-inferred plasmonic activity.

BET/DFT analysis demonstrated mesoporous structures, with dominant pore sizes in the 2–5 nm range and a surface area of 23 m^2/g. Isotherm Type IV profiles with H1 hysteresis loops confirmed interconnected mesopores and capillary condensation effects.

Table 1. Phase composition of Mn-diffused KDB-3 silicon.

Phase	XRD Peak (°2θ)	Phase Presence
SiB_6	29.4, 43.1	Confirmed
Mn_5Si_3	36.7, 41.8	Confirmed
Amorphous Si	Broad halo	Dominant (>70%)

4. Discussion

The collective results underscore that high-temperature manganese diffusion profoundly modifies the structural, phase, and plasmonic characteristics of KDB-3 silicon. The detection of secondary Mn_5Si_3 and SiB_6 phases confirms the thermodynamic tendency of manganese to segregate and form silicide compounds within the silicon matrix during high-temperature processing, as similarly reported by Wang et al. and Ren et al. [12].

The substantial increase in amorphous content (>70%) is noteworthy, as amorphous silicon regions play a critical role in hosting and stabilizing metallic nanoclusters, which act as centers for localized plasmonic oscillations. This finding is consistent with the works of Sun et al. and Bao et al., who emphasized the importance of amorphous-dielectric matrices in enhancing plasmonic responses [1], [13].

Raman and impedance spectroscopy provided complementary evidence of LSPR phenomena. The observed 570–600 cm^{-1} bands in Raman spectra and the 40–70 kHz phase angle minima in impedance plots closely parallel earlier studies on Mn-doped and other transition-metal-modified Si systems by Xie et al., Li et al., and Kobayashi et al. [14]. These results validate the hypothesis that manganese nanoclusters embedded in a silicon matrix can support plasmonic oscillations, thereby expanding the functional possibilities of doped semiconductor systems.

The development of mesoporosity, with pore sizes predominantly between 2–5 nm and a significant increase in surface area (23 m^2/g), not only facilitates the formation of plasmonic active sites but also promotes enhanced charge transport and adsorption properties. This observation echoes conclusions drawn by Thommes et al. and Huang et al., who demonstrated the pivotal role of nanoporosity in modulating both optical and electrical behaviors in doped semiconductor frameworks[15].

Furthermore, the observed fivefold reduction in charge carrier mobility, coupled with increased resistivity, reflects the combined influence of amorphization, defect accumulation, and phase inhomogeneity on electrical transport, consistent with findings by Petrov et al. and Yang et al. [10], [14]. This degradation of carrier mobility suggests potential applications in resistive-type sensors and thermoelectric devices where controlled carrier scattering is advantageous.

Overall, the synergy between multiphase formation, nanostructuring, amorphization, and mesoporosity establishes a conducive environment for plasmonic enhancement, paving the way for multifunctional silicon-based platforms in nanophotonics, sensorics, and spintronics, as proposed by Ma et al. and Sun et al.

5. Conclusion

This research establishes that manganese diffusion at elevated temperatures induces comprehensive structural and plasmonic modifications in KDB-3 silicon. The interplay between phase transformations, amorphous content increase, and mesoporosity development culminates in the manifestation of LSPR phenomena, verified via Raman and impedance spectroscopy.

Modified KDB-3 silicon showcases potential as a multifunctional material in plasmonic sensors, optoelectronic components, and spintronic applications. Future work will focus on broadening the doping temperature range, investigating long-term operational stability, and refining LSPR detection through infrared spectroscopy and photonic correlation techniques.

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