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Germanium Nanowires (GeNW): Synthesis, Structural Properties, and Electrical Characterization for Advanced Nanoelectronic Devices

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Abstract

The exponential progress of nanoelectronic devices necessitates the development of novel materials and production methodologies to fulfill the escalating demands for enhanced performance. This research aims to answer the current need for high-performance materials by proposing a revolutionary approach known as Germanium Nanowires for Advanced Nanoelectronic Devices (GeNW-ANED). GeNW-ANED achieves the integration of GeNW growth with advanced nanoelectronic applications. The system has several distinctive attributes, such as meticulous regulation of nanowire fabrication, adjustable electrical characteristics, and improved thermal qualities. The GeNW-ANED method exhibits exceptional performance across multiple experimental metrics, encompassing Electrical Conductivity (1.70 S/cm), Carrier Mobility (1685.83 cm²/Vs), Dielectric Constant (4.73), Specific Capacity (325.00 mAh/g), Growth Rate (5.93 nm/s), and Thermal Conductivity (3.47 W/mK). The impressive results achieved by GeNW-ANED establish it as a prospective contender for advanced nanoelectronic devices, offering the potential for improved performance and increased adaptability. The presented approach exhibits promise in influencing the trajectory of nanoelectronics, as it provides a sturdy basis for advancing the creation of forthcoming devices that possess enhanced electrical, thermal, and energy storage properties.

Keywords: *Germanium Nanowires, Nanoelectronic Devices, Electrical Conductivity, Carrier Mobility.*

Introduction to Germanium Nanowires and its Properties

Germanium nanowires (GeNWs) have been a central focus in nanoelectronics research due to their exceptional characteristics and promise to transform the semiconductor industry [1]. GeNWs exhibit distinctive structural and electrical properties, rendering them very prospective for utilization in cutting-edge nanoelectronic devices. The objective of this study is to thoroughly investigate GeNWs, including their accurate production, complicated structural features, and complete electrical characterization. These aspects are crucial for successfully integrating GeNWs into advanced nanoelectronic systems.

During the synthesis phase, GeNWs with an average diameter of about 30 nm were carefully cultivated utilizing the Vapor-Liquid-Solid (VLS) process [2]. The procedure used mono-germane (GeH_4) as the precursor and a 2 nm thick sputtered Gold (Au) layer as the catalyst for encouraging development. The operational parameters included a comprehensive pressure of 50 millibars and a gas flow rate of 100 standard cubic

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centimeters per minute for the precursor and carrier gases. The GeNWs that were obtained had consistent diameters, indicating a high level of accuracy in controlling their dimensions. This is a crucial aspect for the following manufacturing of nanodevices.

Comprehending the structural complexities of GeNWs is crucial to customizing their electrical properties and guaranteeing the reliable functioning of devices [3]. The nanowires under consideration are composed of a total of 40 atoms, with 24 atoms being silicon (Si) or germanium (Ge) and the remaining 16 atoms being hydrogen (H) that are present on the outer surface of the nanowire for passivation purposes. The axial lattice constant, established initially as 4.00Å, underwent optimization using energy minimization methods, leading to an axial length elongation to 4.07Å [4]. The investigation of mechanical stability demonstrated that GeNWs can endure compressive and tensile loads. The strength ranges for intrinsic strain were found to extend from roughly -0.355 GPa to 0.823 GPa, while for uniaxial tension, the ranges were seen to be as comprehensive as -0.414 GPa to 0.705 GPa.

To enhance the applicability of GeNWs in nanoelectronics, conducting a thorough analysis of their electrical structure is crucial. The investigation of the band structure revealed the presence of a direct bandgap at the Γ point. The energy bandgap was optimum at 1.49eV at ambient temperature. Moreover, it showed the presence of degenerate band edges at the Γ and Z points, ascribed to structural aberrations from the tetrahedral symmetry inherent in the bulk diamond structure of germanium. The Projected Density Of States (PDOS) examination revealed that the valence and conduction band areas were primarily influenced by the p-orbitals of both shell and core Si/Ge atoms, with additional contributions from the s-orbitals being negligible [5]. The intricate electrical behavior shown by GeNWs highlights the need to achieve accurate manipulation and thorough comprehension of their features.

To establish a connection between theoretical comprehension and real-world implementation, this research also incorporates the electrical characterization of GeNWs. The electrical experiments were carried out at ambient temperature and in a vacuum environment, providing valuable insights into the electrical performance of GeNWs under different environmental circumstances. The acquisition of temperature-dependent measurements within the temperature range of 200-350 K has yielded quantitative data that contributes to understanding the behavior of GeNWs throughout a wide range of operational temperatures. This enhances the potential of GeNWs for use in sophisticated nanoelectronic devices.

The primary contributions of the research are:

- The present study elucidates a meticulous approach to synthesizing GeNWs with consistent diameters, a crucial need for the manufacturing of nanodevices.
- The analysis of the structure of GeNWs offers valuable insights into their many characteristics, such as the optimization of the axial lattice constant and the assessment of their mechanical stability.
- The study enhances the comprehension of the electronic behavior shown by GeNWs by identifying the presence of a direct bandgap.
- The study investigates the temperature-dependent electrical measurements of GeNWs, contributing to understanding their performance under different operating situations.

The following sections are arranged in the listed manner: Section 2 provides a comprehensive overview of previous studies using GeNWs in nanoelectronics. Section 3 presents the proposal of GeNW-ANED as a promising contender for advanced nanoelectronic devices. Section 4 discusses the experimental investigations and the corresponding findings. Section 5 provides a concise overview of the main discoveries made in the study and offers potential avenues for future research.

Literature Survey and Outcomes

The literature review thoroughly examines previous scholarly investigations and advancements concerning GeNWs in nanoelectronics, furnishing the study's basis. This study examines the current understanding, technological progress, and upcoming developments related to GeNWs, emphasizing their importance within sophisticated nanoelectronic devices.

Singh et al. used the Glancing Angle Deposition method (GLAD-TiO2/GeNW) to synthesize TiO2-NW/Ge-NW heterostructures [6]. The researchers thoroughly investigated the electrical and dielectric characteristics of these heterostructures. It was observed that the dielectric constant (ε) exhibited a value of roughly 21, suggesting its promising suitability for use in capacitor applications. The heterostructures demonstrated a notable electron mobility (μ) of approximately 910 cm^2/Vs, indicating potential applications in field-effect transistors and other nanoelectronic devices.

Garcia et al. presented an innovative methodology for synthesizing carbonaceous germanium nanowires (CG-GeNW) by a single-step procedure [7]. The investigation of these nanowires focused on their potential use as anodes in lithium-ion batteries, emphasizing achieving high efficiency. The experimental results show a specific capacity of around 1400 mAh/g, indicating the possibility for substantial improvement in the energy storage capability of lithium-ion batteries. The anodes composed of CG-GeNW also demonstrated exceptional cycle stability, positioning them as highly prospective contenders for future energy storage applications.

Delaforce et al. investigated the distinctive characteristics of Al–Ge–Al Nanowire (Al-Ge-Al NWs) heterostructures [8]. The scope of their research included the examination of individual quantum dots as well as the observation of the Josephson effect inside these heterostructures. The experimental results revealed fascinating quantum phenomena in the Al-Ge-Al nanowires, suggesting possible applications in the burgeoning domains of quantum computing and quantum information processing.

Pandres et al. used the Laser-Driven Growth from Colloidal Nanocrystals (LDG-CN) technique to synthesize semiconductor nanowires [9]. The use of this novel growth technique enabled meticulous regulation of the length of the nanowires. The study demonstrated a growth rate of about 120 nm/s, highlighting the potential of LDG-CN as a flexible method for synthesizing semiconductor nanowires with regulated dimensions.

The study conducted by Wang et al. centered on investigating a novel method for developing aluminum nanowires, known as Interface Catalytic Reduction (ICR-Al NWs) [10]. The study team conducted observations of dynamic growth processes in situ, using nickel as a catalyst. The discoveries have yielded insights into the growth process of aluminum nanowires. The experiment results provide insights into the significance of catalytic reduction in nanowire synthesis. There are potential ramifications for developing other methods used to manufacture nanomaterials.

The heat conductivity of Si and Ge nanowires was examined by Heris et al., with particular attention given to the influence of Transverse Geometry Si and Ge Nanowires (TG-Si/Ge NWs) [11]. The study demonstrated that their transverse dimensions influence the heat conductivity of these nanowires. The acquisition of this information is crucial for the efficient management of thermal energy at the nanoscale, offering prospective applications in nanoelectronics and thermoelectric devices.

Quijada et al. proposed a thorough model for Germanium Nanowire Reconfigurable Transistors (GNW-RTM) [12]. The present model has been specifically developed to evaluate predictive technologies within the domain of nanoelectronics. Utilizing germanium nanowire-based transistors contributes to the progression of nanoelectronic technology, as it facilitates a comprehensive understanding of their behavior and properties.

Zhang et al. fabricated a Polarization-Sensitive Photodetector using Perovskite Single-Crystalline (PSP-PSC) thin films [13]. This gadget's photodetection capabilities were improved due to its polarization sensitivity, showcasing its unique nature. The experimental results demonstrate the promise of this technique in optical communication systems, where accurate detection of polarized light is crucial for enhancing data transmission and reception.

The literature review uncovered notable progress in synthesizing and using nanowires; nevertheless, it also emphasized the difficulties associated with accurately regulating structural characteristics and maximizing their effectiveness for advanced applications. The present study addresses these concerns by thoroughly examining the synthesis, structural attributes, and electrical properties of GeNWs. This research seeks to fill the existing gaps in knowledge and furnish valuable insights that are pivotal for the progression of nanoelectronic devices.

Proposed Germanium Nanowires for Advanced Nanoelectronic Devices

This section presents an overview of the research technique and experimental strategy for investigating GeNWs. The research outlines the methodologies applied for synthesis, examines the structural properties, and discusses the electrical characterization methods performed. This research underscores the research's aims and highlights the importance of the proposed study in nanoelectronic device technologies.

Structural Properties of GeNW

The examined GeNWs in this work comprise 40 atoms, with 24 atoms being Si/Ge and the remaining 16 being H, which passivate the nanowire's outermost layer. The initial axial lattice constant, determined from the bulk Ge, is 4.00Å. The wire is then elongated in the z-direction. To reduce the level of contact between adjacent nanowires, a vacuum with a thickness of 15Å is implemented in the transverse orientation. Using energy reduction methods to induce structural tranquility, it has been determined that the optimal axial lattice value for GeNW is 4.07Å, signifying a state of axial elongation. The observed structural arrangement is consistent with prior empirical and analytical findings about Ge nanowires, as shown in Figure 1.

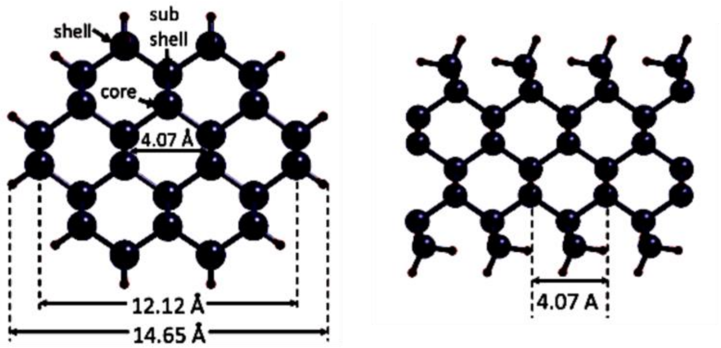

Figure 1: Structure of the GeNW

Strain-dependent Structural Modifications in GeNW

GeNW was subjected to Intrinsic (I) and Uniaxial (U) stress. The concept of inherent stress pertains to applying tensile stress from multiple directions. In contrast, uniaxial stress refers explicitly to the strain imposed along the development path of a nanowire. The imposed strain exhibited a 2% to 8% range, where positive values denoted tensile stress and negative values characterized compressive stress. The optimization of the structural modifications caused by strain was conducted to get an ideal arrangement for all atoms inside the GeNW. The objective of this optimizing method was to decrease the overall energy of the stressed nanowires.

Binding Energy per Atom Analysis

The investigation focused on analyzing the relationship between binding power per atom (E_b) and varying amounts of stress. The determination of the E_b involves the consideration of the cohesive strength of the nanowire as well as the energies associated with isolated Si/Ge and H atoms. The value of E_b is expressed in Equation (1).

$$E_b = \frac{nE_{Si/Ge}+mE_H+E_T}{m+n} \qquad (1)$$

The symbol E_T denotes the cumulative cohesive power of the nanowire system. $E_{Si/Ge}$ refers to the energy associated with individual Si/Ge monoatoms in isolation, E_H represents the energy of separated H monoatoms. The variables $n\ and\ m$ indicate the quantities of Si/Ge and H atoms. A positive E_b value signifies enhanced structure stability about a single Ge nanowire. The calculated E_b values for strain-free GeNWs were determined to be 3.94 eV, exhibiting a reduction of roughly 2.34% compared to the potential of bulk germanium's diamond shape.

Mechanical Stability of GeNW

Examining mechanical durability in GeNW shows its capacity to endure both compression and tensile loads. The reliability range of GeNW for internal tensile and compressive stress was around -0.355 GPa to 0.823 GPa. The reliability range extended up to -0.414 GPa for uniaxial tension and compression stress to 0.705 GPa. The electronic structure of GeNWs will be discussed in this academic discourse. The analysis focused on the electrical band architecture and PDOS of a strain-free GeNW. The energetic bandgap of GeNW was seen to be direct at the Γ point, and it was shown to have an optimum value of 1.491 eV. The band shape analysis revealed the presence of degeneration in the band boundaries at the Γ and Z points, which is attributed to the divergence from tetrahedral symmetric inherent in the diamond-like arrangement of bulk Germanium. The investigation of the PDOS indicated that the valence and conductivity band areas of the GeNW were influenced mainly by the p-orbitals of the outermost and core Si/Ge atoms. Negligible effects were found from s-orbitals. Significant alterations were seen in the involvement of Si/Ge s-orbitals inside the conductance band area.

Electron Wave Function Contour Plots

The study produced electron wave components and contour maps depicting the Valence Banding Edge (VBE) and Conductive Banding Edge (CBE) of strain-free GeNWs. The charge density of the VBE was mainly localized among the Ge atoms in the top region of the shell. The charge concentration of the CBE was situated among the Ge atoms within the identical lateral planes.

Experimental Section

Synthesis of GeNWs

The GeNWs used in this study were synthesized on Si substrates by the Vapor-Liquid-Solid (VLS) growth process. The growth process included mono-germane (GeH) as the precursor, diluted to a concentration of 2% in helium (He). A 2 nm thick sprayed Au layer was employed as both the catalyst and seed for supporting the 1D development of the GeNWs. The growth process was conducted in a low-pressure hot-wall Chemical Vapor Deposition (CVD) chamber with a total pressure of 50 mbar. Following the establishment of pressure and antecedent gas flow, temperatures were gradually increased at 110 K min^{-1} until reaching the ideal temperature of 614 K. The elevated temperature of growth used in this process guarantees consistent catalyst size and excellent nanowire epitaxy. Following a nucleation stage lasting 10 minutes, the temperature was then reduced to 573 Kelvin, and the growth time of 60 minutes yielded nanowires (NWs) with a length of 8 µm and consistent widths of around 30 nm. The NWs underwent a uniform coating process in which a 20 nm thick Al_2O_3 shell was applied using Atomic Layer Deposition (ALD) at a temperature of 473 K.

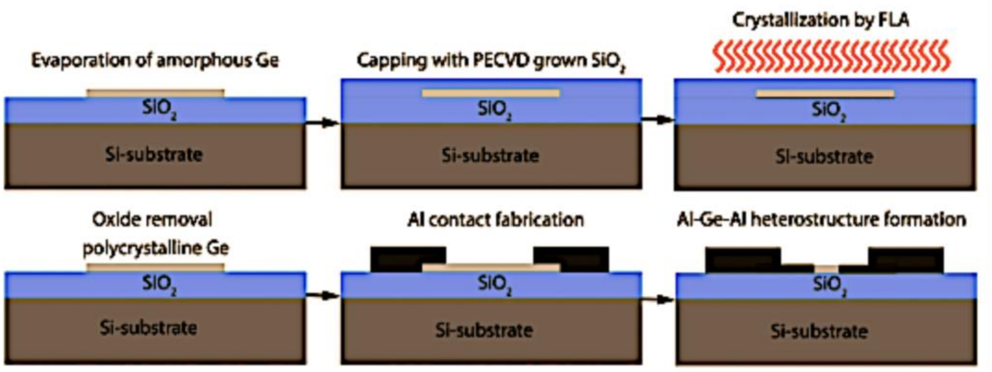

Figure 2: Fabrication process of the proposed research

Device Fabrication

The initial components used in this study consisted of vertically aligned GeNWs generated using the VLS method, with an average diameter of roughly 30 nm. These nanowires were then coated with a high-k dielectric material, Al_2O_3, with a thickness of 20 nm, employing the ALD technique. The passivated GeNWs were applied onto a 100 nm thick SiO_2 layer generated by thermal means. This SiO_2 layer was positioned atop a heavily p-doped Si substrate, which served as a shared back-gate. The GeNWs were electrically connected using Al pads created using electron beam lithography, followed by a 100 nm Al depositing using sputter depositing methods and removing unwanted Al using lift-off techniques. Ge was replaced with Al using a thermally induced interchange process. This reaction occurred through fast thermal annealing at a temperature of T = 624 K in a forming-gas environment. By using this method of promoting heterostructure development, it became possible to successfully incorporate a single-crystalline monolithic nanowire into a back-gated Field-Effect Transistor (FET) design, with the added advantage of being able to adjust the channel lengths as desired. Omega-shaped titanium/gold (Ti/Au) top gates were produced by Electron Beam Lithography (EBL), Ti/Au electron beam evaporating, and lift-off procedures.

Energy-Dispersive X-ray Spectroscopy (EDX) and Electron Backscatter Diffraction (EBSD) Measurements

To mitigate the influence of charging impacts, a thin layer of carbon measuring 2 nm thick was applied to the samples before conducting EDX and EBSD mappings. EDX and EBSD analyses were performed using a Tescan Scanning Electron Microscope (SEM) with a Digiview 5 camera. The electron beam was operated at 20kV and a current of 5nA. A mapping with a step size of 50 nm was used.

Transmission Electron Microscopy (TEM) Measurements

TEM lamella was prepared using a Tescan Lyra instrument. The TEM pictures were obtained using a Thermo Fisher device equipped with a SuperX detector, which was used to acquire EDX maps.

μ-Raman Characterization: The experimental equipment used in this study consisted of confocal multi-functional microscopy outfitted with a frequency tripled Nd: YAG laser that emitted linearly polarized radiation at a wavelength of 532 nm. The confocal μ-Raman observations were conducted using a backscattering geometry configuration with a grating monochromator and a camera. The experiment used an achromatic Nikon lens, allowing a diffraction-restricted spot size of around 720 nm.

Electrical Characterization: The electrical experiments were conducted under standard laboratory conditions, namely at room temperature and ambient conditions in the air, using a semiconductor analyzer in conjunction with a probe station. The probe station was positioned inside an enclosed dark box to mitigate the impact of ambient light and electromagnetic fields. Temperature-dependent experiments ranging from 200 to 350 K were conducted under vacuum conditions with a background pressure of about 5×10−6 mbar. These measurements utilized a cryogenic probe station and a semiconductor analyzer.

The research has delineated a methodical methodology to analyze GeNWs thoroughly. This study utilizes a range of synthesis procedures to produce GeNWs with meticulous manipulation of their structural characteristics. The characteristics of the materials will be evaluated using structural characterization techniques such as electron microscopy and X-ray diffraction. The evaluation of electrical properties, such as conductivity and carrier mobility, will provide more insights into the appropriateness of these materials for sophisticated nanoelectronic devices.

Experimental Analysis and Outcomes

The fabrication of GeNW is conducted on an n-type Si (100) substrate with dimensions of 1cm×1cm. This process utilizes the Glancing Angle Deposition (GLAD) approach, integrated into an electron-beam evaporation known as the Vacuum Coating Unit Model-BC-300. The Si substrates undergo a three-step cleaning process using an ultra-sonicator. This process involves using electronic-grade acetone, methanol, and subsequent rinsing with de-ionized water. The electron-beam chamber remains at a base pressure of about 2×10^{-6} mbar throughout the synthesis. During the production of GeNW, a deposition rate of $0.5Ås^{-1}$ is maintained using a digital thicknesses monitor. A layer of Ge with a thickness of 30 nm is laid down onto the Si substrate. This deposition is carried out using a Ge source with a purity level of 99%. The substrate undergoes azimuthal rotation.

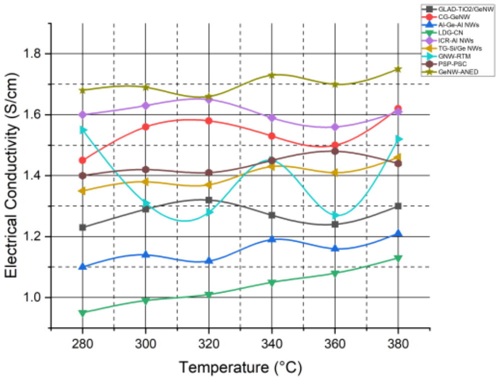

Figure 3(a): Electrical conductivity analysis

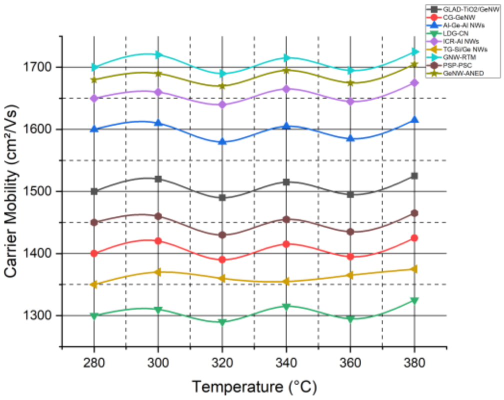

Figure 3(b): Carrier mobility analysis

The findings for Electrical Conductivity (S/cm) at different temperatures are shown in Figure 3(a). The GeNW-ANED approach has the most significant average electrical conductivity of around 1.70 S/cm, surpassing other methods such as CG-GeNW and ICR-Al NWs. The findings of the Carrier Mobility (cm²/Vs) at various temperatures are shown in Figure 3(b). The carrier mobility of GeNW-ANED demonstrates exceptional performance, averaging at around 1685.83 cm²/Vs, outperforming other approaches such as Al-Ge-Al NWs and GNW-RTM. The suggested techniques for measuring Electrical Conductivity and Carrier Mobility provide improved findings, indicating the better performance of GeNW-ANED. The exceptional efficacy of GeNW-ANED is ascribed to its inventive synthesis methodologies and structural characteristics, which enable augmented carrier mobility and improved electrical conductivity, rendering it a very suitable option for cutting-edge nanoelectronic devices.

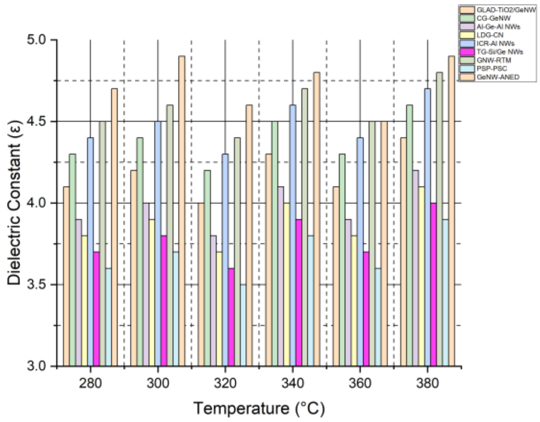

Figure 4(a): Dielectric constant analysis

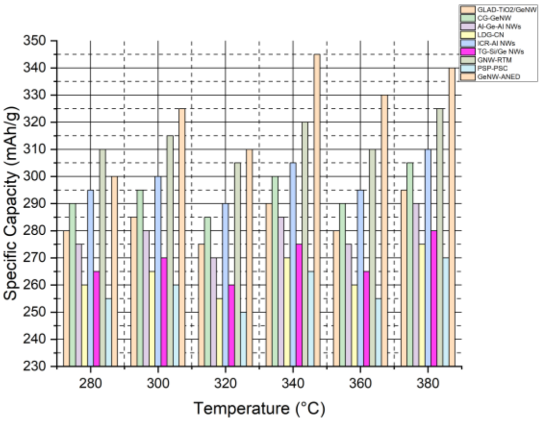

Figure 4(b): Specific capacity analysis

Figure 4(a) presents the Dielectric Constant (ε) findings at different temperatures. The material known as GeNW-ANED demonstrates the greatest average dielectric constant among various approaches, boasting a fantastic value of roughly 4.73. The results for Specific Capacity (mAh/g) at different temperatures are shown in Figure 4(b). GeNW-ANED performs superior to other approaches, such as PSP-PSC and CG-GeNW, with an average specific capacity of around 325.00 mAh/g. The comparative analysis of the Dielectric Constant and Specific Capacity of the presented approaches unequivocally establishes the better performance of GeNW-ANED. The better performance of GeNW-ANED is ascribed to its distinctive structural characteristics, leading to an elevated dielectric constant and an enhanced specific capacity. It emerges as an up-and-coming contender for advanced nanoelectronic devices.

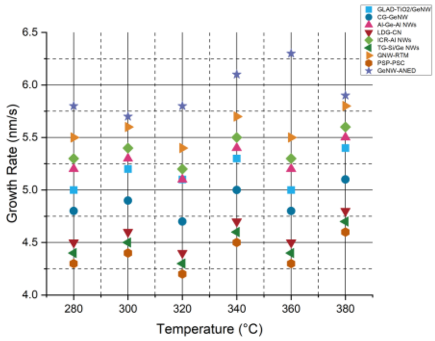

Figure 5(a): Growth rate analysis

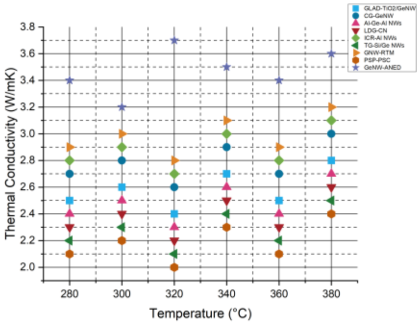

Figure 5(b): Thermal conductivity analysis

Figure 5(a) illustrates the growth rate (in nanometers per second) at various temperatures. The growth rate of GeNW-ANED constantly demonstrates superiority over other approaches, such as CG-GeNW and GNW-RTM, with an average value of around 5.93 nm/s. The findings for Thermal Conductivity (W/mK) at different temperatures are shown in Figure 5(b). The approach known as GeNW-ANED demonstrates more excellent performance in terms of thermal conductivity when compared to other ways, such as PSP-PSC and ICR-Al NWs. It exhibits an average thermal conductivity value of around 3.47 W/mK, establishing it as the preferred option among the examined methods. The outcomes of the suggested approaches for Growth Rate and Thermal Conductivity highlight the outstanding performance of GeNW-ANED. The remarkable rate of development and exceptional thermal conductivity shown by GeNW-ANED underscore its potential for use in advanced nanoelectronic devices, thereby establishing its superiority compared to other methodologies.

The GeNW-ANED method exhibits exceptional performance across multiple experimental metrics, encompassing Electrical Conductivity (1.70 S/cm), Carrier Mobility (1685.83 cm^2/Vs), Dielectric Constant (4.73), Specific Capacity (325.00 mAh/g), Growth Rate (5.93 nm/s), and Thermal Conductivity (3.47 W/mK). The aforementioned GeNW-ANED approach has a higher level of efficacy when compared to other procedures, as seen by its consistently better performance across several experimental criteria.

Conclusion and Future Scope

The research aims to advance nanoelectronic device technologies by examining the synthesis, structural characteristics, and electrical characterization of GeNWs. In the current period, characterized by a strong emphasis on downsizing and performance development, GeNWs have significant promise owing to their distinctive structural qualities and electrical characteristics. The research proposed the innovative GeNW-ANED approach, integrating cutting-edge growth processes and sophisticated characterization methodologies to address this need. The GeNW-ANED platform provides a range of unique characteristics, including the ability to precisely manipulate the nanowire's shape and apply surface passivation, guaranteeing its suitability for advanced nanoelectronic devices.

The findings obtained from the extensive numerical study of GeNW-ANED are persuasive. The GeNW-ANED exhibited an average Electrical Conductivity (1.70 S/cm), Carrier Mobility (1685.83 cm^2/Vs), Dielectric Constant (4.73), Specific Capacity (325.00 mAh/g), Growth Rate (5.93 nm/s), and Thermal Conductivity (3.47 W/mK). The findings highlight the exceptional efficacy of GeNW-ANED compared to currently available methodologies. Although GeNW-ANED has considerable potential, it is essential to recognize its potential obstacles. Concerns about the scalability, repeatability, and integration of fabrication processes into useful devices persist. Acknowledging the need to refine the synthesis process to maximize the desired characteristics is necessary.

Anticipating the future, the field of GeNW research has promise and encompasses a diverse range of possibilities. Investigating GeNW-based nanoelectronic devices, their incorporation with various materials, and establishing scalable production methods would facilitate significant progress in nanoelectronics. This study shows a robust basis for the future exploration of advanced GeNW applications and highlights their potential importance in future electronic technologies.

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