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Research Article

THEORETICAL ANALYSIS FOR ENHANCING PERCOLATION CHARACTERISTIC IN NANOMATERIALS DESIGN

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Abstract

Recent advances in strategies for soft materials have drawn attention for developing wearable and bioelectronics, transitioning them from rigid to soft systems. This shift offers significant advantages, particularly in mechanical compatibility with human tissues. Among these materials, conductive nanocomposites stand out as essential components, serving as conductive interconnects in stretchable electronic systems. Despite notable progress, optimizing conductive nanocomposites to enhance performance while preserving their mechanical properties remains a significant challenge.In this study, we explore the key parameters influencing the performance of conductive nanocomposites through both qualitative and quantitative analyses. We begin by summarizing recent advancements in metallic nanocomposites and then delve into the three-dimensional percolation theory, which provides a theoretical foundation for understanding the random systems of nanocomposites. Additionally, we identify critical parameters that can modulate the percolative connections of nanoparticles inside of soft elastomer matrix. Finally, we discuss the potential applications of optimized conductive nanocomposites, with a focus on wearable and bio-implantable systems. The article concludes with a brief summary and a discussion of the remaining challenges in this field.

Keywords: Percolation Theory, Conductive nanocomposite, Nanomaterial, Conductive pathway, Wearable sensor.

INTRODUCTION

Elastic and deformable electronics have been in high demand due to their capacity for creating wearable and comfortable electronic devices. For instance, essential components such as sensors (1), actuators (2), energy harvesters (3), and circuits (4) have been engineered in stretchable forms to meet the requirements of wearable and bio-implantable systems. Consequently, materials tailored to match the qualities of these components have been extensively researched, including ultrathin metal/oxide films (5) and wavy or serpentine thin metals (6). However, while these materials meet the demands for mechanical durability and sturdiness, their inherent brittleness and rigidity make them unsuitable for applications requiring mechanical compatibility with human tissues, such as organs and skin. To address this challenge and develop electronic systems that minimize mechanical mismatches between biotic and abiotic interfaces, researchers have focused on nanocomposites, which are fabricated by incorporating elastic polymers and metallic nanomaterials. Stretchable nanocomposites one of the most promising candidates for intrinsically stretchable electronics consist of a polymer matrix, functional nanoparticles, and an organic medium. These materials offer exceptional mechanical properties, such as elasticity and stretchability, making them ideal for applications requiring seamless integration with human tissues. To further enhance their suitability for human-friendly devices, researchers are actively investigating ways to optimize nanocomposites to achieve superior electrical performance without compromising their mechanical integrity. In this work, we highlight key advances in the development of stretchable and conductive nanocomposites, with a particular emphasis on material synthesis and the interplay between mechanical and electrical performance. We analyze the theoretical frameworks and parameters that govern the electrical behavior of these materials. Specifically, we explore recent advancements in metallic nanocomposites, focusing on strategies that enhance conductivity. Using insights derived from the study of parameters such as three-dimensional percolation theory, which describes the connectivity of conductive nanoparticles, we establish qualitative and quantitative relationships between these parameters and the resulting material properties. Finally, we discuss the practical applications of optimized conductive nanocomposites in wearable and bioelectronic systems, underscoring their potential to bridge the gap between rigid electronics and soft, human-compatible interfaces.

Why dowe need conductive nanocomposites in flexible/stretchable electronics?

The demand for conductive nanocomposites in flexible and stretchable electronics stems from the transformative shift in electronic systems from rigid, planar configurations to dynamic, deformable platforms that seamlessly integrate with non-traditional surfaces, including the human body. Conventional rigid materials, such as silicon and metal films, are fundamentally incompatible with the requirements of wearable and bio-implantable devices due to their limited flexibility, high brittleness, and inability to conform to complex, curved surfaces. These limitations have driven a significant push toward the development of materials that combine the electrical functionality of traditional conductors with the mechanical properties of elastomers. Conductive nanocomposites, composed of conductive nanofillers embedded in elastic polymer matrices, have emerged as a promising solution, offering unique advantages that address the challenges posed by the mechanical and electrical demands of next-generation electronic systems. A key reason for adopting conductive nanocomposites is their ability to maintain electrical conductivity under large mechanical deformations. Devices used in wearable and bioelectronic applications

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frequently undergo dynamic and repeated stresses, including bending, stretching, and twisting. Traditional conductive materials fail in these scenarios, as they crack or delaminate under strain, leading to electrical failure. In contrast, nanocomposites leverage conductive nanofillers such as carbon nanotubes, graphene, metallic nanoparticles, and nanowires, which form interconnected networks within a soft, elastic polymer matrix. These networks provide percolative pathways for electron transport while allowing the composite to deform elastically. This intrinsic stretchability ensures that the electrical performance of the nanocomposites remains stable, even under extreme strain, making them indispensable for applications requiring high mechanical compliance. Another critical need for conductive nanocomposites arises from their ability to minimize mechanical mismatch between electronic systems and biological tissues. Human tissues, such as skin, muscles, and organs, exhibit low modulus values and are inherently soft and deformable. For wearable electronics or bio-implantable devices to function effectively and comfortably, they must exhibit similar mechanical properties to avoid irritation, tissue damage, or device failure. Rigid electronics are prone to causing mechanical stress at the interface with soft tissues, which can lead to delamination or discomfort during use. Conductive nanocomposites, with their tailored elasticity and softness, provide a mechanically compatible interface that allows electronic devices to adhere conformally to skin or internal organs, ensuring user comfort and enhancing device functionality. Conductive nanocomposites also address the growing need for lightweight and multifunctional materials in modern electronics.

The incorporation of nanofillers enables not only high electrical conductivity but also additional functionalities, such as thermal conductivity, electromagnetic shielding, and sensing capabilities. For example, composites containing graphene or carbon nanotubes can simultaneously conduct electricity, dissipate heat, and detect strain or pressure, reducing the need for separate components (7). This multifunctionality is particularly beneficial in space-constrained applications, such as wearable health monitors or implantable medical devices, where compact and efficient designs are essential. From a manufacturing perspective, conductive nanocomposites offer significant advantages in terms of processability and scalability. Unlike traditional electronic materials, which often require high-temperature or vacuum-based processes, nanocomposites can be fabricated using solution-based techniques such as casting, printing, or spraying (8). These methods are not only cost-effective but also compatible with large-scale production, enabling the commercialization of stretchable electronic devices. Additionally, nanocomposites can be tailored to achieve desired electrical and mechanical properties by adjusting parameters such as filler type, loading, and dispersion, providing unparalleled flexibility in design and application. The growing interest in the Internet of Things (IoT) and wearable technologies further underscores the necessity of conductive nanocomposites. As devices become increasingly interconnected and portable, there is a need for flexible materials that can withstand daily wear and tear without sacrificing performance. Conductive nanocomposites meet this requirement, enabling the development of wearable devices that monitor health parameters, power themselves through energy harvesting, and communicate wirelessly with external systems. These capabilities are driving innovation in healthcare, fitness, and consumer electronics, creating a demand for materials that combine reliability with adaptability. In summary, the need for conductive nanocomposites in flexible and stretchable electronics stems from their ability to address the limitations of traditional materials while unlocking new possibilities for device functionality and integration. Their unique combination of electrical conductivity, mechanical compliance, multifunctionality, and processability makes them indispensable for a wide range of applications, from wearable sensors and medical implants to energy storage devices and electronic skins. As research in this field continues to advance, conductive nanocomposites are poised to play a central role in shaping the future of soft and human-compatible electronics.

Recent progresses in metallic nanocomposite

General metals are often stiff and bulky, making them incompatible with soft electronics, which are typically attached on skin. However, metallic nanomaterials address this issue by enabling the creation of stretchable or flexible composite materials. These nanomaterials exhibit unique electrical, thermal, and magnetic properties derived from their dimensions. Like bulk metals, metallic nanomaterials possess exceptional electrical and thermal conductivities. When mixed with an elastic polymer, they form conductive nanocomposites that are both soft and conductive. Within this soft matrix, metallic nanomaterials create conductive pathways based on a percolation network, enabling effective electrical conductivity while retaining mechanical flexibility. Metallic nanomaterials can be categorized by their dimensions, including 0D (nanoparticles), 1D (nanowires), and 2D (nanosheets) structures (Figure 1). Zero-dimensional (0D) metallic nanomaterials, such as gold, palladium, silver, and platinum nanoparticles, have been extensively explored. However, constructing a conductive percolation network solely with 0D nanomaterials remains challenging as their shape is not advantageous to form network. To overcome this limitation, 0D nanomaterials are often combined with 1D and 2D counterparts to enhance electrical conductivity without compromising the mechanical properties of the composite (9). Two-dimensional (2D) nanomaterials, such as nanosheets or flakes, are particularly advantageous for forming conductive pathways due to their larger contact area, which facilitates better connectivity between fillers compared to the point contacts provided by 0D and 1D nanomaterials. Consequently, 2D nanomaterials are frequently used in conductive nanocomposites. To further improve conductivity and mechanical properties, 0D nanomaterials are often incorporated into 1D and 2D systems, creating hybrid filler materials that optimize both electrical and mechanical performance.Soft conductive nanocomposites incorporating 0D, 1D, and 2D metallic nanomaterials have demonstrated promising applications. For instance, Kim and colleagues fabricated a stretchable conductor composed of gold nanoparticles (AuNPs) and a polyurethane (PU) matrix. Citrate-stabilized AuNPs, with sizes ranging from 8 to 13 nm, were integrated into the PU matrix using two techniques: layer-by-layer (LBL) deposition and vacuum-assisted flocculation (VAF). Both methods resulted in nanocomposites with identical filler content (21.7% by volume). Mechanical and electrical properties of the films were analyzed, revealing their potential for high-performance stretchable conductors (10).In another study, Oh et al. developed a conductive composite with remarkable elongation properties. By combining methyl isobutyl ketone (MIBK), stretchable rubber, and silver (Ag) flakes, they achieved a composite capable of stretching up to 400% before breaking. They used flashinducing sintering process to make better connection between metal nanomaterials. Such composite material demonstrated potential applications in wearable sensor technologies (11). Moreover, researchers have shown that the electrical performance of conductive nanocomposites, which degrades under high strain, can be recovered through dynamic rearrangement of nanofillers within the matrix (12).These advancements highlight the versatility and potential of metallic nanomaterials in developing soft conductive composites. By leveraging the unique properties of 0D, 1D, and 2D nanomaterials, researchers continue to push the boundaries of stretchable electronics, paving the way for innovative applications in wearable devices, sensors, and beyond.

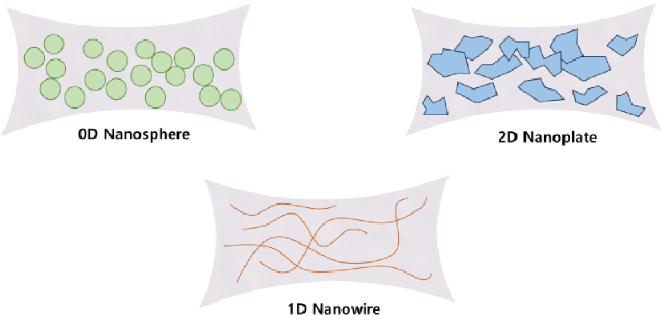

Figure 1. Schematic showing the nanocomposite with different shapes of nano fillers

Three-dimensional percolation theory for designing the nanocomposite materials

Three-dimensional (3D) percolation theory is a fundamental concept used to understand and optimize the behavior of composite materials, particularly in terms of their electrical, thermal, and mechanical properties. This theory describes the transition from an insulating to a conductive state in a composite system when conductive fillers are dispersed within an insulating matrix. Percolation occurs when a critical concentration of fillers, known as the percolation threshold, is reached, allowing the formation of a continuous conductive network throughout the material. Understanding and applying 3D percolation theory is crucial for designing high-performance composites, as it directly impacts their functionality and efficiency in applications such as electronics, sensors, and energy storage devices. In a composite material, the spatial distribution and connectivity of conductive fillers, such as metallic nanowires, carbon nanotubes, graphene, or nanoparticles, determine the percolation behavior. In three dimensions, the percolation threshold depends on several factors, including the shape, size, aspect ratio, and orientation of the fillers, as well as their interactions with the matrix material. Fillers with higher aspect ratios, such as 1D nanowires or 2D nanosheets, typically require lower concentrations to form a conductive network due to their greater likelihood of overlapping and forming pathways. This is particularly advantageous in applications where maintaining the mechanical flexibility of the composite is critical, as lower filler loadings minimize the stiffening effects on the matrix. Percolation theory in three dimensions also considers the randomness of filler placement and connectivity. Statistical models, such as Monte Carlo simulations, are often employed to predict the percolation threshold and the properties of the composite. These models account for the stochastic nature of filler dispersion and provide insights into the design of composites with tailored properties. For example, achieving a uniform distribution of fillers is essential to ensure consistent conductivity and mechanical performance across the composite. Beyond the threshold, the electrical conductivity of the composite follows a power-law relationship, which is described by the critical exponent associated with the percolation transition. This relationship allows researchers to predict how changes in filler content or distribution influence the composite's performance. In classical percolation theory, researchers typically assume a well-defined geometrical criterion for inter-element bonding, enabling the determination of the minimal concentration of bonds required to form a connected network, known as the percolation threshold. Such systems are observed in various porous media and complex polymer matrices, characterized in the continuum by a critical fractional volume of nanomaterials, denoted as V_c. The value of V_c can range from nearly zero to the close-packing limit of the corresponding nanomaterials, as illustrated in Figure 2.Near the percolation threshold, the electrical conductivity of a composite follows a power-law relationship as shown in Equation 1:

$$\sigma=\sigma_0(V_f-V_c)^S \quad \text{(Equation 1)}$$

where σ is the electrical conductivity of the composite, σ_0 is the electrical conductivity of the filler, V_f is the filler volume fraction, V_c is the percolation threshold, and S is the conductivity exponent. However, Equation 1 does not account for factors such as shape of particle, their orientations, polymer-particle interactions, or particle dispersion. Consequently, the values of S and $V_c$are not constants but vary depending on the specific composite system. These parameters must be determined experimentally through curve fitting of measured data. The conductivity exponent S and the critical volume fraction V_c are intrinsic properties of the nanomaterial and polymer system. Beyond the basic equation, numerous geometric and physical factors can influence the value of S, including the shape of the nanomaterials, the density of the polymer chains, and the degree of filler dispersion. We will discuss the effects of these parameters in detail in the following section.

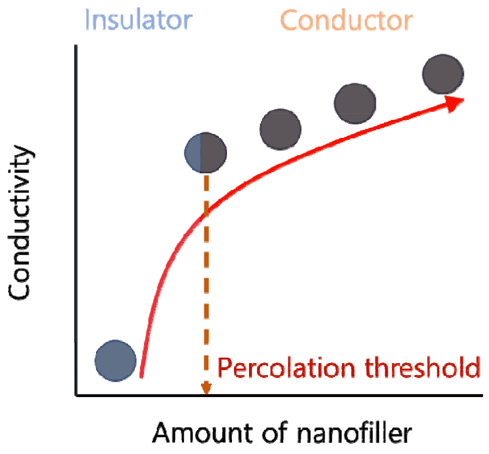

Figure 2. Conceptual graph showing percolation threshold, termed V_c

Effect of geometrical factor in conduction pathways

To design the efficient nanocomposite design, we can use various kinds of conductive nanomaterials having different shapes such as 0D, 1D, 2D, and 3D. The spatial distribution of fillers in unit volume is important to anticipate the percolation characteristics. To examine the effect of geometry, this section evaluates 2D and 3D randomly distributed platelets, with a specific focus on the influence of the geometric shape of the platelets. We assumed 2D structures to be plates and 3D structures to be spheres, respectively. To establish the relationship between the nanomaterial volume fraction and other parameters, the distance between adjacent conductive particles is calculated. It is assumed that the particles are homogeneously distributed and fixed within a unit cubic polymer matrix. In case of spherical particle, we could express the *L* and $V_f$as below (Figure 3a)

$$L = D + I = \sqrt[3]{\frac{\pi D^3}{6V_f}},\ V_f = \frac{V_{nano}}{L^3} \quad \text{(Equation 2)}$$

where *D* and $V_f$are the diameter and the volume fraction of particle, *I* is the distance between particle. Volume fraction of nanoparticle can be expressed as volume ratio between nanoparticle and unit cubic-shaped matrix. Rearranging equation 2 gives below (Equation 3).

$$V_f = \pi \frac{D^3}{6(D+I)^3} \text{(Equation 3)}$$

The critical volume fraction of spherical particles in a composite depends on the particle diameter and the distance between particles. Using this relationship, the required volume fraction of spherical nanoparticles to establish conductive connections can be estimated.

In case of 2D square-like nanoplate (Figure 3b), we assume that there is no angle variance. From this assuption, we can also express the V_f as a function of *D* and *I*in the similar way with spherical nanoparticle as below shown in Equation 4 and 5.

$$L = D + I = \sqrt[3]{\frac{tD^2}{V_f}},\ V_f = \frac{V_{nano}}{L^3} \quad \text{(Equation 4)}$$

$$V_f = \frac{tD^2}{6(D+I)^3} \text{(Equation 5)}$$

From these calculations, we can estimate the minimum amount of conductive nanofiller for making percolation network inside of polymer matrix.

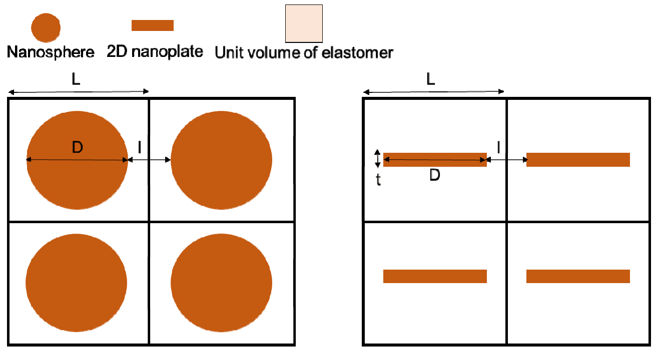

Figure 3. Schematic showing model of composite in different shape of nanomaterials

Potential applications of conductive nanocomposite

Conductive nanocomposites, which combine electrically conductive nanomaterials with a flexible matrix, have emerged as promising materials with a broad range of potential applications across various industries, due to their unique combination of electrical, mechanical, and thermal properties. One of the most prominent applications of conductive nanocomposites is in flexible and stretchable electronics. These materials are ideal for fabricating devices that must retain electrical performance while being bent, stretched, or deformed, making them critical in the development of wearable technologies, such as smart watches, flexible displays, and e-skin. In particular, conductive nanocomposites can be used to create stretchable circuits, interconnects, and antennas, enabling the development of next-generation electronics that maintain durability and performance even when subjected to mechanical strain (13). Additionally, conductive nanocomposites are crucial in wearable sensors for health monitoring, where they are embedded in textiles or patches to monitor vital signs such as heart rate, body temperature, and blood glucose levels (14). These sensors rely on the high sensitivity and flexibility of nanocomposites, which can detect minute changes in resistance caused by mechanical deformation, making them ideal for real-time health tracking. Another key area of application is in energy storage and conversion devices, where conductive nanocomposites are utilized in flexible batteries, supercapacitors, and fuel cells. By improving the electrical conductivity of electrodes, these materials enhance the performance, capacity, and flexibility of energy storage devices, enabling more efficient and lightweight solutions for portable and wearable electronics (15). Conductive nanocomposites also play a crucial role in electromagnetic interference (EMI) shielding, offering lightweight and flexible alternatives to traditional shielding materials. These composites are highly effective at absorbing and dissipating electromagnetic radiation, making them ideal for protecting sensitive electronic devices in communication systems, automotive electronics, and aerospace applications. With the rapid expansion of wireless technologies and the growing demand for compact electronic devices, EMI shielding materials are becoming increasingly vital for maintaining signal integrity and ensuring device functionality (16). In the biomedical field, conductive nanocomposites are paving the way for advanced medical devices and implants. Their biocompatibility and electrical conductivity make them suitable for applications like neural interfaces, which restore or enhance nerve function, and electroactive scaffolds for tissue engineering, which promote cell growth and regeneration (17). In conclusion, conductive nanocomposites are rapidly advancing across multiple fields, driving innovation in wearable electronics, energy storage, healthcare, environmental monitoring, and more. Their versatility in combining conductivity with mechanical flexibility opens new possibilities for next-generation technologies that are more efficient, sustainable, and adaptable. As research in this area continues to grow, we can expect to see even more groundbreaking applications that will shape the future of materials science and engineering.

Conclusion

In conclusion, enhancing the percolation characteristics in nanomaterial design is critical for optimizing the electrical conductivity and mechanical properties of composite materials. Theoretical analysis plays aimportant role in understanding the relationship between nanomaterial geometry, filler concentration, and the percolation threshold. By considering factors such as particle shape, distribution, and the nature of interactions between the nanofillers and the matrix, we can refine design strategies for improving conductivity in nanocomposites. The incorporation of multi-dimensional nanomaterials such as 0D, 1D, and 2D structures offers promising avenues for achieving lower percolation thresholds and enhancing the overall performance of conductive composites. Moreover, the integration of hybrid nanomaterial systems, combining multiple dimensionalities, holds potential for creating more efficient and mechanically stable conductive networks. While significant progress has been made in the theoretical understanding of percolation theory and its application to nanocomposite design, further research is necessary to fully comprehend the complex factors influencing conductivity and to develop tailored nanomaterials that meet the demands of next-generation technologies in fields like electronics, energy storage, and biomedical applications. Ultimately, advancing the theoretical framework for percolation in nanomaterials will continue to guide the development of high-performance materials with enhanced conductivity and functionality.

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