Thermoplasmonics Decontamination of Respirators Face Masks Using Silver Nanoparticles: A New Weapon in the Fight Against COVID-19 Pandemic

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Abstract
The current COVID-19 pandemic has resulted in an urgent need for methods to decontaminate respirators masks for reuse while keeping them intact and functional. The severe shortage of professional masks such as N95 and FFP2 has necessitated their reuse over long periods. A very promising method is the pasteurization of these masks by thermoplasmonic heat generated by plasmonics nanoparticles when they are irradiated by light. Under illumination at its plasmonic resonance, a metal nanoparticle features enhanced light absorption, turning it into an ideal nano-source of heat, remotely controllable using light. In this work, we propose a numerical study based on the finite element method (FEM) of the thermoplasmonic properties of silver nanoparticles (AgNPs) decorating polypropylene (PP) fibers which is a basic material for the manufacture of these masks. The surface plasmon resonance (SPR) of these nanostructures was investigated through the computation of the complex effective dielectric permittivity and the absorption cross section in the near UV–visible (NUV-Vis) range. First, the SPR characteristics of AgNPs for different morphologies are determined from the absorption spectra, including the SPR-peak position $\lambda_{\text{max}}$ and the electric field enhancement. Second, we determine the power absorbed by an individual AgNP of different morphologies. From this, we calculate the internal temperature increase of the particle at the plasmonic resonance. The last step is devoted to the determination of the temperature profile in the surrounding medium in order to better understand and design the plasmon-assisted heating processes at the nanometric scale.

Keywords Thermoplasmonics · Polypropylene fibers · Nanocomposites · Metallic nanoparticles · Finite element method

Introduction
Respirator mask is an essential part of personal protective equipment during times of infectious disease. Although respirators are intended for single use, high demand during a pandemic like COVID-19 has forced healthcare providers to reuse respirators. Based on the manufacturer’s instructions, they are heat sensitive and not designed to be sterilized; however, due to their high costs and limited availability [1, 2], different methods to decontaminate N95 and FFP2 [3–7] respirators have been discussed to allow multiple usages. Decontamination methods can be classified into chemical or physical treatment, dry heat, or moist heat [8]. Recommendations suggest that masks should pass the verification test; the filtering capacity of the masks must remain the same; and no residue from the decontamination process should remain [2, 8]. Developing a self-decontamination method by integrating sterilizing agents into the textile threads of these masks is of crucial importance. A wide variety of commercial medical masks are made of polypropylene (PP) non-woven fabric with three different layers. While the outer layer filters large particles, the middle layer is a filter media for fine particles and the third layer is a direct contact skin layer. The studies have focused on the performance of commercial medical mask and N95 respirators [9, 10]. These studies revealed that N95 respirators sometimes failed to
provide 95% protection level against airborne viral agents and some surgical masks allowed the penetration of significant fraction of airborne viruses. The lack of performance of medical masks forced the global researchers to think about high-performance, reusable medical masks for the safety of both public and medical workers. One of the strategies to achieve this objective is to either modify surface of the fabric or apply a protective coating over the fabrics used in commercial face mask [11, 12]. Another milestone in this area is the generation of a photo sterile mask by the utilization of photothermal effects of nanomaterials [13]. The self-sterile properties along with super hydrophobic nature of these surfaces make the mask more effective to stop the spreading of COVID-19 [14].

Silver nanoparticles decorating the surface of fibrous materials can be utilized for their intrinsic bactericidal and antiviral activities, thus enabling an active methodology for minimizing the accumulation of harmful and living pathogens in the PP fiber pores [15]. The antiviral mechanism of AgNPs is based on the binding of these NPs to the viral genome, thereby blocking the activity and interaction of various viral and cellular factors responsible for replication, resulting in the inhibition of viral replication and the release of virions from the progeny [16]. In this regard, AgNPs have antiviral activity against human immunodeficiency virus-1 (HIV-1) [17], herpes simplex [18], and respiratory syncytial virus [19]. Silver exhibits low toxicity to human cells, and silver has a lower propensity to induce microbial resistance than many other antimicrobial materials [20, 21]. As a result, AgNPs have been applied to a wide range of products, such as in burn and traumatic wound dressings, diabetic ulcers, coating of catheters, dental works, scaffold, and medical devices [20, 22]. In addition, AgNPs have high photothermal efficiency, possessing an absorption spectrum in the near UV–visible (NUV-Vis) band, which can be used to trigger light-assisted photothermal disinfection [23]. Indeed, the ability of AgNPs to convert a monochromatic light into thermal energy (photothermal effect) has marked their utilization in several pathogenic diseases’ treatments through the so-called photothermal therapy (PTT) [24]. The photothermal conversion in AgNPs due to a phenomenon called local surface plasmon resonance (LSPR) [25–27]. In this effect, the incident photons, colliding with metallic nanoparticles, can cause free electrons to corporately oscillate under proper conditions known as plasmon oscillation [28]. When the frequency of this collective oscillation matches with the incident light frequency, it establishes the resonance called surface plasmon resonance (SPR). Under this SPR resonance condition, optimal light can be harvested from the different parts of the solar spectrum for different application purposes. The resonance frequency depends on the size, shape, and material composition of the nanostructure. Since the absorbed energy will be released as heat to the environment, plasmonic NPs can serve as light-to-heat converters. One important advantage of a plasmonic nanostructure is that heating can be triggered and controlled by external irradiation, for instance, by a laser. The interaction between a nanoparticle and an incoming light can be described by two parameters: the scattering and absorption cross sections. While the scattering cross section tells how light will be re-radiated by the nanoparticle, the absorption cross section is directly related to heat generation. Thus, absorption is what primarily matters in thermoplasmonics, the domain of nanoplasmonic that uses plasmonic nanoparticles as nano-sources of heat [29–31].

The absorption cross section of a plasmonic nanoparticle embedded in the surrounding medium can be evaluated by considering the whole as a matrix-inclusion nanocomposite. The effective dielectric permittivity of a nanocomposite is an essential parameter influencing the absorption of light by the medium. The effective permittivity describing the relationships between the microscopic and macroscopic properties of composites has been described by many analytical and theorical methods, called effective medium theory (EMT); these are the famous formulas of Clausius Mossotti (CM), Maxwell–Garnett (MG), and Rayleigh [32, 33]. Numerical techniques are designed to solve the relevant filed equation in the computational domain, subject to the boundary constraints imposed by the geometry. Without making a priori assumption about which field interaction is most significant, numerical techniques analyze the entire geometry provided as input. The finite element method (FEM) [34], which is a powerful numerical modeling tool, has been widely used for modeling electromagnetic wave interaction with complex materials [35–37].

In this paper, we use the FEM to determine the electric potential distribution in a nanostructure consisting of AgNPs deposited on PP non-woven fibers or confined between two fibers. This calculation method allowed us to compute the real and imaginary parts of the effective dielectric permittivity and the absorption cross section in the NUV-Vis spectral range. The SPR properties of AgNPs are determined from the absorption peak which allows the determination of the thermoplasmonic power dissipation in the surrounding medium at the resonance.

The remaining of presentation is organized as follows. The principle of the numerical method (FEM) is illustrated in the “Numerical Method” section. Afterwards, we describe the physics of heat generation in metal NPs in the “Physics of Plasmonic Heating” section. Then, we present the numerical results and discussions in the “Results and Discussion” section. Finally, some concluding remarks are drawn in the last section.
Numerical Method

Polypropylene (PP) fiber is one of the most widely used synthetic fibers in the textile industry. PP has some advantages: it is cheaper and stronger than other synthetic fibers. Besides, it is well applicable for various fields; in particular, it is used for sanitary applications such as respirator protection masks, diapers, filters, and hygienic bands, which need to display antibacterial effects [38, 39]. The integration of AgNPs in PP fibers in respirator face masks has a double interest for the fight against the pandemic COVID-19. It is known that silver is one of the safer antibacterial agents when compared to organic compounds [40]; silver has been medically proven to kill over 650 disease-causing organisms in the body. They also have the advantage to generating heat at the nanometric scale by the SPR phenomenon induced by the absorption of light which allows to decontaminate their environment by the thermoplasmonic heat. In this work, we are interested in the numerical study using FEM of SPR properties and thermoplasmonic heat generation of silver nanoparticles decorating PP fibers in non-woven textiles of respiratory masks as shown in Fig. 1. In this textile, the AgNPs can be seen in two more frequent configurations, either
deposited on the PP fiber away from the other fibers or confined between two fibers as shown in Fig. 2. For these configurations, the optical response of AgNPs to an incident electromagnetic ( electromagnetic wave) depends on the direction of the wave vector \( \mathbf{k} \) with respect to the fiber orientation; the direction incidence of the electromagnetic wave is determined by the angle \( \theta \) (see Fig. 2).

To illustrate the FEM, we consider a three-dimensional structure composed of \( L \times L \times L \) cubic cells to simulate the inclusion and matrix elements. The inclusion (AgNPs) elements are placed randomly in the matrix material. The presented structure is used to calculate the effective permittivity of two-phase disordered composites with the concentration of inclusions \( f = 0.05 \).

Considering absence of charge density in the composites, numerical solutions of electrostatic problems in a material are based on the solutions of Laplace's equation:

\[
\nabla (\varepsilon_0 \varepsilon (\mathbf{r}) \nabla V(\mathbf{r})) = 0
\]

where \( \varepsilon(\mathbf{r}) \) and \( \nabla V(\mathbf{r}) \) are the local relative permittivity and the potential distribution inside the material domain respectively, and \( \varepsilon_0 = 8.85 \times 10^{-12} \text{F/m} \) is the permittivity of the vacuum. FEM is used to solve the equation and obtain the electric filed distribution in the composite. The material is exposed to a static electric field, which is generated by a voltage across the opposite faces of the cube, and the other faces of the cube meet the requirement of \( \partial V/\partial n = 0 \). By dividing the domain into finite elements, the calculation of the potential distribution for each element is carried out by interpolation of the potential \( V \) and its normal derivative \( \partial V/\partial n \) with the corresponding nodes [41, 42]:

\[
V = \sum \lambda_i V_i
\]

(2)

\[
\frac{\partial V}{\partial n} = \sum \lambda_i \left( \frac{\partial V_i}{\partial n} \right)
\]

(3)

where \( \lambda_i \) denotes the interpolating functions. Once the potential distribution is known, the effective permittivity of a composite is calculated by the energy balance method. The electrostatic energy \( W_e \) and losses \( P_e \) for each element can be expressed as:

\[
W_e^k = \varepsilon_0 \int \frac{1}{2} \left( V_k^p \right)^2 \left[ \left( \frac{\partial V_k}{\partial x} \right)^2 + \left( \frac{\partial V_k}{\partial y} \right)^2 + \left( \frac{\partial V_k}{\partial z} \right)^2 \right] \, dV_k
\]

(4)

\[
P_e^k = \frac{1}{2} \omega \varepsilon'' \int \left( \frac{\partial V_k}{\partial x} \right)^2 + \left( \frac{\partial V_k}{\partial y} \right)^2 + \left( \frac{\partial V_k}{\partial z} \right)^2 \, dV_k
\]

(5)

where \( \varepsilon_k \) and \( V_k \) represent the permittivity and the volume of the \( k \)th tetrahedron element, respectively. The total electrostatic energy \( W_e \) and losses \( P_e \) in the entire composite can be calculated by summation of all the elements. On the other hand, the composite material can be regarded as a capacitor that stores the electrostatic energy when it is exposed to the electric field. The stored electrostatic energy and losses in the capacitor can be calculated macroscopically by:

\[
W_e = \frac{1}{2} \varepsilon_{\text{eff}} \frac{S_d}{L} (V_2 - V_1)^2
\]

(6)

\[
P_e = \frac{1}{2} \omega \varepsilon''_{\text{eff}} \frac{S_d}{L} (V_2 - V_1)^2
\]

(7)

where \( V_1 \) and \( V_2 \) are the potentials applied across to plates of the unit cell. Here, \( S_d \) is the surface of in-depth. From the evolution of the effective complex dielectric function depending on the wavelength (or frequency) of the incident field, the resonance modes that may occur in AgNPs are identified. For this, it would be interesting to calculate the scattering cross sections and absorption; the sum of these two quantities defines the extinction cross section

\[
\sigma_{\text{ext}} = \sigma_{\text{abs}} + \sigma_{\text{diff}}
\]

(8)

In the case where the dimensions are very small compared to the wavelength, the light scattering can be ignored, and we have: \( \sigma_{\text{ext}} \approx \sigma_{\text{abs}} \). The absorption cross section can be determined from the imaginary part of the effective dielectric function of the composite using the following equation [43, 44].

\[
\sigma_{\text{abs}} = \frac{V_p}{f} \frac{k}{n_{\text{eff}}} \varepsilon''_{\text{eff}}
\]

(9)

Here, \( V_p \) stands for the common volume of nanoparticles, \( f \) is their fraction, \( k \) is the wave vector amplitude of the electromagnetic wave, and \( n_{\text{eff}} \) represents the refractive index.

**Physics of Plasmonic Heating**

Metallic nanostructures such as AgNPs support electronic resonances known as SPR that can be excited upon illumination. The frequency of SPR strongly depends on the morphology of the metal nano-object and its dielectric environment. The SPR is an efficient way to confine energy into the extremely small volume of an AgNP, thus drastically enhancing both its absorption and scattering cross sections [45]. The absorption cross section specifies the portion of absorbed light that is reemitted in the form of heat; therefore, absorption is what primarily matters in thermoplasmonics [46].
In the interaction with an impinging short light pulse in the UV–Vis–NIR spectral domain, the AgNPs can gain energy by absorbing photons through electron transitions. After the absorption of the photon energy by the metallic NP the internal energy of the electron gas passes through the following: (1) a rapid and resonant enhancement (SPR); (2) a confined electron gas redistribution through electron–electron collisions (e–e); (3) a fast decrease with the electron–phonon scattering (e–ph); and (4) a slow recovery of the initial state of equilibrium via phonon–phonon-collisions (ph–ph) (heat transfer to the surrounding medium). The total amount of thermal energy generated by a single AgNP must equal the amount of thermal energy generation (which accounts for the Joule effect), plus the thermal energy confined inside the AgNP. To describe the local temperature profile inside and around AgNPs embedded in a dielectric medium, we use a heat transfer equation [47].

\[
\rho C_p \frac{\partial T(r)}{\partial t} = \nabla \cdot \left( \kappa \nabla T(r) \right) + q(r) \tag{10}
\]

where \( \rho \) and \( C_p \) are the density and specific heat capacity at constant pressure, respectively, \( T(r) \) is the absolute temperature, and \( \kappa \) is the thermal conductivity of the surrounding medium; \( q(r) \) is the external source of heat in the medium, here the heating generated by the AgNP. In the steady-state regime, when the local temperature reaches its equilibrium profile, i.e., \( \frac{\partial T(r)}{\partial t} = 0 \), this equation reduces to,

\[
\nabla \cdot \left( \kappa \nabla T(r) \right) = -q(r) \tag{11}
\]

Assuming \( \kappa \)-values for silver and surrounding medium are noted \( \kappa_A \) and \( \kappa_m \) respectively, Eq. (11) can be split into two parts: \( \kappa_A \nabla^2 T(r) = -q(r) \), inside the AgNP, and \( \kappa_m \nabla^2 T(r) = 0 \), outside the AgNP. For a spherical AgNP of radius \( R \), simple calculations lead to a temperature increase [48]:

\[
\delta T(r) = \delta T_{NP} \frac{R}{r}, r > R, \tag{12}
\]

\[
\delta T(r) \approx \delta T_{NP}, r < R, \tag{13}
\]

where \( \delta T_{NP} \) is the temperature increase of the NP. The power absorbed (and delivered) by a AgNP can be simply expressed using the absorption cross section \( \sigma_{abs} \) introduced in the previous section: \( Q = \sigma_{abs} \cdot I \), where \( I \) is the irradiance of the incoming light (power per unit surface) [49]. The temperature variation \( \delta T_{NP} \) of a uniformly charged AgNP surrounded by a homogeneous medium and possessing a thermal conductivity \( \kappa_m \) is given by:

\[
\delta T_{NP} = \frac{Q}{4\pi\kappa_m R} = \frac{\sigma_{abs} \cdot I}{4\pi\kappa_m R} \tag{14}
\]

For non-spherical NPs, there is no simple analytical expression giving the NP temperature increase \( \delta T_{NP} \) as a function of the absorbed heat power \( Q \) and numerical simulations are required. However, Baffou et al. [48] proposed to use a dimensionless geometrical correction factor \( \beta \) defined such that the NP temperature increase reads:

\[
\delta T_{NP} = \frac{\sigma_{abs} \cdot I}{\beta 4\pi\kappa_m R_{eq}} \tag{15}
\]

where \( R_{eq} \) is the equivalent NP radius. The values of \( \beta \) for a large set of geometries with axial symmetry (namely rods, ellipsoids, discs, and tori) are given in reference [48].

**Results and Discussion**

**Optical Properties**

In this work, the optical and thermoplasmonic properties of the outer layer of a respiratory face mask consisting of a nanocomposite AgNPs/PP fiber are investigated using the finite element method. The optical properties of silver nanoparticles in the ultraviolet and visible (NUV-vis) domains are governed by the collective response of conduction electrons. These form an electron gas that moves away from its equilibrium position when perturbed by an external light field, thus creating induced surface polarization charges that act as a restoring force on the electron gas. This results in collective oscillatory motion of the electrons which is characterized by a dominant resonance band lying in the NUV-Vis for silver. The far-field performance of the nanoparticles is summarized in the wavelength-dependent absorption \( \sigma_{abs} \) and scattering cross sections \( \sigma_{sca} \), which are defined as the effective area of a screen with which the incoming light interacts (by absorption or scattering) in a straight-ray picture. Indeed, the interaction between a suitable light source and an AgNP produces absorption and scattering of the incident radiation, thus generating a light attenuation characterized by an extinction cross section \( \sigma_{ext} \). For small AgNPs (size \( \ll \lambda \)), \( \sigma_{ext} \) strictly depends on the absorption process:

\[
\sigma_{sca} \ll \sigma_{abs} \approx \sigma_{ext}. \tag{16}
\]

Classical electromagnetic solutions provide an excellent description of the optical properties of silver nanoparticles, with silver represented by its bulk, frequency-dependent dielectric function \( \varepsilon(\omega) \), as determined from optical measurements in macroscopic films. In this work, the dielectric function of AgNPs describes the three-critical point Drude model (three-CPDM) [50]. It should be noted that this model gives a good approximation of the dielectric function of silver which is valid for wide frequency band between 0.6 and 6.87 eV corresponding to wavelengths between 181 and...
2069 nm. The optical characterization of PP fibers can be determined by UV–visible and dielectric spectroscopy. Here, we used the experimental results obtained by Ben Ammar and Fakhfakh [51], these authors determined the optical and dielectric properties of PP fibers at room temperature by UV–visible spectroscopy in the spectral range between 200 and 800 nm.

In the AgNPs/PP fiber nanocomposite, the optical response of Ag nanoparticle following a light irradiation depends on the configuration of the particle with respect to the PP fibers and on the incidence direction with respect to the fiber orientation. We consider here two possible configurations: (i) AgNP deposited on the PP fiber far from the other fibers, (ii) AgNP confined between two parallel fibers. The direction of incidence of the light varies between two extreme cases, an incidence perpendicular or parallel to the orientation of the fiber. Figure 3a and b show the evolution of the absorption cross section of AgNP of radius $R = 10$...
nm deposited on the PP fiber in NUV-Vis frequency band (between 250 and 500 nm) for different values of the light intensity: Fig. 3a, when the incidence direction of light is normal to the fiber orientation, i.e., the incident electric field $\vec{E}_0$ is parallel to the fiber, and Fig. 3b, when the incidence is parallel to the fiber, i.e., the incident field is normal to the fiber direction. These curves show that the absorption spectrum of the AgNPs/PP fiber nanocomposite exhibits a maximum for a specific wavelength $\lambda_{\text{max}}$ which corresponds to the SPR peak of the AgNP. This resonance peak is located at $\lambda_{\text{max}} = 365$ nm when the incidence light is perpendicular to the fiber and at $\lambda_{\text{max}} = 380$ nm when the irradiation direction is parallel to the fiber. These curves also show that for both incidence directions the light absorption by the metal nanoparticle increases when the light intensity increases.

We have plotted in Fig. 4a and b the absorption spectra of AgNP confined between two PP fibers for the two directions of propagation of the electromagnetic wave: normal (Fig. 4a) and parallel (Fig. 4b). The SPR peak position does not change compared to the first configuration (at 365 nm

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**Fig. 4** Absorption cross section spectra of AgNP confined between two PP fibers in the case of normal (a) and parallel (b) incidence light for different values of the light intensity.
for normal incidence and at 380 nm for parallel incidence). In this case, the absorption cross section also increases by increasing the light intensity. These curves show that the confinement of the metal nanoparticles between the PP fibers causes an increase in the absorption at the SPR but has no effect on the shift of the SPR peak position. Furthermore, the direction of incidence of light influences the amount of light absorbed by the AgNP and the SPR peak position. These results are explained by the fact that when the collective vibrations of the electric charges at the plasmonic resonance take place towards the metal–dielectric interface, the absorption is very strong.

**Optical Heating and Temperature Profile of AgNP**

Finding the most suitable thermoplasmonic nanoparticle for a specific application is not a easy step as it often takes into consideration several factors that can be physical, chemical, or biological in nature. To accomplish this task, it is necessary to adapt the following parameters: the nanoparticle size,
its shape, its composition, and its environment. A common goal for all applications of thermoplasmonics is to maximize light-to-heat conversion of the nanoparticles. This can be first achieved by increasing the size of the nanoparticles, by modifying their morphology, or by adjusting the direction of light incidence in the case of anisotropic nanostructures. The quantum efficiency of noble metals being low, we can consider that the totality of the energy absorbed by the NP will be converted into heat. Remarkably, such a rationale explains why noble metals are more efficient plasmonic materials and remain, after two decades, the preferred plasmonic materials for both optical and thermal experiments. The heat induces an increase in the temperature of the nanoparticle (\(\delta T_{NP}\)) which locally heats the surrounding medium. Since metals have high thermal conductivity, the temperature of the NP is expected to be homogeneous in the nanoparticle. The plasmonic heat depends on the absorption cross section of the nanoparticle which is described by the relation (14). The

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**Fig. 6** Internal temperature variation spectra of AgNP confined between two PP fibers and irradiated by an electromagnetic wave in the 250–500-nm band for normal (a) and parallel (b) irradiation.
absorption cross section $\sigma_{abs}$ scales indeed as the volume (V) of the nanoparticle, at least for small nanoparticles in the quasistatic regime (for instance, for silver nanospheres typically smaller than 60 nm). Normalizing $\sigma_{abs}$ by the nanoparticle volume leads to a refined figure of merit that isolates the effect of shape and composition, as it no longer depends on the nanoparticle size (at least for small nanoparticles). On the other hand, as we have shown above, the absorption cross section of AgNP depends on the configuration of the surrounding medium and on the direction of the exciting light for anisotropic structures, which necessarily influences the amount of converted energy into heat.

Figure 5a and b show the plots of the local temperature change $\delta T_{NP}$ of AgNP in the frequency band 250–500 nm for different values of the light intensity which varies from 20 to 100 mW/cm². These curves are obtained for an AgNP deposited on a PP fiber as a function of the radial coordinate for different values of light intensity, normal (a) and parallel (b) irradiation.
of radius \( R = 10 \text{ nm} \) deposited on a PP fiber for the two extreme cases of the incident light direction, normal to the fiber direction (electric field \( \vec{E}_0 \) is parallel) (Fig. 5a) and parallel to the fiber direction (electric field \( \vec{E}_0 \) is perpendicular) (Fig. 5b). These curves show that the temperature of the particle increases sharply in the SPR band around the wavelength \( \lambda_{\text{max}} \) which is due to the conversation of light energy into heat; on the other hand, far from plasmonic band, the temperature of the particle is equal to that of their environment. When the light intensity varies from 20 to 100mW/cm², the temperature change in the particle increases from \( \delta T_{\text{NP}} = 0.85\,^\circ\text{C} \) to \( \delta T_{\text{NP}} = 9.52\,^\circ\text{C} \) for normal incidence and from \( \delta T_{\text{NP}} = 4.86\,^\circ\text{C} \) to \( \delta T_{\text{NP}} = 54.36\,^\circ\text{C} \) for parallel incidence. These results show that when the incident electric field is perpendicular to the fiber direction (wave vector \( \vec{k} \) is parallel to the fiber orientation), there is a strong confinement of the oscillating electric charges at the SPR which leads to a strong conversation of the energy into heat. Figure 6a and b show the plots of the temperature change in the particle when it is confined between two PP fibers for the two cases of light incidence directions, normal (Fig. 6a) and parallel (Fig. 6b). The obtained results show that when the light intensity varies from 20 to 100mW/cm², the local temperature change in the particle varies from \( \delta T_{\text{NP}} = 1.32\,^\circ\text{C} \) to \( \delta T_{\text{NP}} = 14.84\,^\circ\text{C} \) for the normal incidence and from \( \delta T_{\text{NP}} = 5.72\,^\circ\text{C} \) to \( \delta T_{\text{NP}} = 63.94\,^\circ\text{C} \) for the parallel incidence.

Upon illumination, the free charges of AgNP oscillate at the frequency of the electric field of the incident light. This electronic oscillation, which is nothing but an electronic current in a metal, generates energy dissipation via the Joule effect. In the case of an isolated AgNP, only the temperature rise due to its own absorption is to be taken into account. Far from the NP, it is equivalent to a heat point source. The heat diffusion will only depend on the power it absorbs. Several approaches of thermoplasmonics are based on a modulated heating of metal nanoparticles using a modulated laser intensity for the measurements of thermal diffusivity [52].

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Several approaches of thermoplasmonics are based on a modulated heating of metal nanoparticles using a modulated laser intensity for the measurements of thermal diffusivity [52]. Such a system raises questions about the amplitude of the nanoparticle’s temperature modulation, its phase delay compared to the light modulation and the spatiotemporal evolution of the temperature distribution in the surrounding medium. In the rest of this section, we shall study the heating dynamics of a single AgNP of radius \( R \) embedded in a PP non-woven tissue. If one considers the inner temperature of the nanoparticle as uniform, the physical quantities of interest in this problem are the temperature change distribution in the surroundings \( \delta T(r, t) \) for \( r > R \) and the temperature change of nanoparticle \( \delta T_{\text{NP}}(t) = \delta T(r = R, t) \). The latter equality comes from temperature continuity considerations at the nanoparticle interface. It is not a simple closed-form expression which exists for the spatiotemporal evolution of the temperature of the system following the absorption of a pulse of light. Numerical simulations have to be conducted. The problem can be simplified by considering the initial temperature change profile \( \delta T(r, 0) \) as uniform (equals \( \delta T_{\text{NP}}(0) \)) inside the nanoparticle since the electron–phonon thermalization usually occurs much faster than the external heat diffusion. Then, one can also suppose that the nanoparticle temperature remains uniform during the evolution of the system because the thermal conductivity of the nanoparticle is much larger than the thermal conductivity of surrounding medium. The equations governing the temperature field are previously described by formulas (12–15).

Figure 7a and b show the profiles’ plots of the temperature change in the vicinity of a AgNP deposited on PP fiber and irradiated by a light pulse of wavelength \( \lambda_{\text{max}} = 365 \text{ nm} \) which corresponds to the SPR. These temperature changes are plotted as a function of radial coordinates for different values of light intensity \( I_0 \) with fixed particle size at \( R = 10 \text{ nm} \). Figure 7a is obtained for normal incident light to the fiber direction (\( \vec{E}_0 \) parallel) and Fig. 7b for parallel incident (\( \vec{E}_0 \) normal). The temperature change inside \( \delta T_{\text{NP}} \) the particle \( r < |R| \) is uniform because the metal particle conductivity is very high. This change is worth between \( \delta T_{\text{NP}} = 0.85\,^\circ\text{C} \) and \( \delta T_{\text{NP}} = 9.52\,^\circ\text{C} \) for a normal incidence and between \( \delta T_{\text{NP}} = 4.86\,^\circ\text{C} \) to \( \delta T_{\text{NP}} = 54.36\,^\circ\text{C} \) for a parallel incidence when the light intensity increases from 20 to 100mW/cm². In the surrounding medium the temperature distribution decreases when moving away from the particle. The radial temperature distribution can be modeled by an exponential law of the following form:

\[
\begin{align*}
\delta T(r) &= \delta T_{\text{NP}} \quad : r \leq R \\
\delta T(r) &= \delta T_{\infty} + Ae^{-\alpha r} \quad : r > R
\end{align*}
\] (16)

where \( \alpha \) is a universal constant that equals to \( \alpha = 0.067 \), \( \delta T_{\infty} \) is a characteristic temperature reached when \( r \geq 10R \), \( [\delta T_{\infty} = \delta T(r \approx 10R)] \), and \( A \) is a constant dependent on light intensity and on the polarization direction and light intensity. In Table 1, we summarize the values of \( \delta T_{\infty} \) and \( A \) corresponding to Fig. 7a and b.

### Table 1

| \( I_0 \) (mW/cm²) | Normal incidence | Parallel incidence |
|------------------|------------------|---------------------|
| \( \delta T_{\infty} \) | \( A \) | \( \delta T_{\infty} \) | \( A \) |
| 20               | 0.11             | 1.36               | 0.61             | 7.75             |
| 40               | 0.30             | 3.84               | 1.73             | 21.92            |
| 60               | 0.56             | 7.06               | 3.18             | 40.27            |
| 80               | 0.86             | 10.87              | 4.90             | 62.00            |
| 100              | 1.20             | 15.19              | 6.85             | 86.66            |
Surface plasmons are electromagnetic modes confined to the metal/dielectric interface (AgNP/PP fiber). They are associated with a collective oscillation of the free electrons of the metal particle which results in a confinement of the optical plasmonic modes in an ultrathin volume. This confinement will lead to an enhancement of the electromagnetic field in very small spaces formed at the AgNP/PP fiber interface. The AgNP/PP fiber interface depends on the arrangement of the nanoparticle in relation to its surrounding PP fiber tissue. Figure 8a and b show the radial distribution of the temperature change of AgNP confined between two PP fibers at the SPR. These curves show that the AgNP produces a greater heating of the surrounding environment when it is confined between two PP fibers compared to the
Table 2 Parameters related to the function (16) modeling the temperature distribution of AgNP confined between two PP fibers when the irradiation is normal or parallel to the fiber

| $I_0$ (mW/cm²) | Normal incidence | Parallel incidence |
|----------------|------------------|-------------------|
|               | $\delta T_\infty$ | $A$               | $\delta T_\infty$ | $A$               |
| 20             | 0.17             | 2.11              | 0.72             | 9.12              |
| 40             | 0.47             | 5.99              | 2.04             | 25.79             |
| 60             | 0.87             | 11.00             | 3.74             | 47.37             |
| 80             | 1.33             | 16.92             | 5.77             | 72.93             |
| 100            | 1.87             | 23.66             | 8.06             | 101.93            |

Fig. 9 Plasmonic temperature profile of AgNP deposited on a PP fiber (a) and confined between two PP fibers (b) as a function of the radial coordinate for different values of the light incidence angle.
Conclusions

In this work, we have studied the optical and thermoplasmonic properties of composite nanostructures consisting of AgNPs embedded in a non-woven tissue of PP fibers. This material can be the basis for the construction of protection face masks to fight against transmissible respiratory diseases that are caused by organisms such as viruses or bacteria that attack the respiratory system such as COVID-19. We used a numerical approach based on FEM to determine the effective dielectric permittivity of the nanocomposite, the effective absorption cross section, and the thermoplasmonic heat generated by the AgNPs at the plasmonic resonance. The SPR properties are identified by the absorption spectra in the NUV-Vis frequency band (250–500 nm) which is the sensitive range for Ag surface plasmons.

Our study also focuses on the effect of nanoparticle configuration with respect to its PP fiber environment. Two configurations are studied: (i) the AgNP is deposited on a single isolated fiber, (ii) the AgNP is confined between two PP fibers. Another parameter that affects the plasmonic properties of the particle is the polarization direction of light with respect to the fiber direction, in this context, we studied two extreme cases, where the incident direction is normal and parallel to the fiber orientation for the two configurations. We have shown that the SPR peak position is located at \( \lambda_{\text{max}} = 365 \) and 380 nm respectively when the incident field \( \vec{E}_0 \) is parallel (wave vector \( \vec{k} \) normal) and \( \vec{E}_0 \) normal (\( \vec{k} \) parallel) to the fiber direction in the two studied configurations. The obtained results show that the light intensity does not affect the SPR peak position; moreover, the amplitude absorption increases when the light intensity increases. The effect of the polarization direction of the incident light on the SPR peak position is studied by considering the angle \( \theta \) between the incident direction \( \vec{k} \) and the fiber orientation, \( \theta = 0 \), corresponds to the parallel incidence, i.e., the incident field \( \vec{E}_0 \) is normal and \( \theta = \pi/2 \) corresponds to the normal incidence (\( \vec{E}_0 \) parallel). Our results show that when \( 0 \leq \theta \leq \pi/4 \), the SPR peak position is located at \( \lambda_{\text{max}} = 380 \) nm and when \( \pi/4 < \theta \leq \pi/2 \), the SPR peak located at \( \lambda_{\text{max}} = 365 \) nm.

The thermoplasmonic power calculations show that the temperature change \( \Delta T_{\text{NP}} \) inside the AgNP increases sharply when it is irradiated at the SPR frequency which is due to the conversation of the light energy into heat. This temperature increase is enhanced in the case of the first configuration compared to the second and in the case when the incident field \( \vec{E}_0 \) is normal to the fiber direction compared to the case when it is parallel. The thermoplasmonic heat of the particle will be dissipated into the surrounding medium; the temperature change profiles are plotted as a function of the radial coordinate \( r \) which represents the distance between the particle center and the point under consideration in medium. The use of AgNPs as a heat source in PP tissues can be used to heat the outer layer of face masks by light; this is a kind of thermal and durable decontamination that can protect individuals during exposure to pests like COVID-19.

The thermoplasmonics field is a recent and growing discipline that has applications in many scientific fields. While metal nanoparticles have long been used primarily for their optical properties, they have recently raised many expectations to improve heat-induced processes in areas such as medical therapy, imaging in biology, hydrodynamics, and chemistry. This diversity stems from the ubiquity of heat-induced effects in all fields of science. This richness is the hallmark of theremoplasmonics, which has become a driving force for creating synergies between different scientific disciplines over the last two decades.

Author Contribution A. Akouibaa: conceptualization, methodology, software, investigation, validation, formal analysis, no funding acquisition, writing—original draft preparation, writing—reviewing and editing, supervision, project administration. R. Massour: conceptualization, methodology, software, investigation, validation, formal analysis, no funding acquisition, writing—original draft preparation, writing—reviewing and editing, supervision, project administration. M. Benhamou: conceptualization, methodology, software, investigation, validation, formal analysis, no funding acquisition, writing—original draft preparation, writing—reviewing and editing, supervision, project administration. A. Derouiche: conceptualization, methodology, software, investigation, validation, formal analysis, no funding acquisition, writing—original draft preparation, writing—reviewing and editing, supervision, project administration.

Data Availability No data availability statement.

Declarations

Conflict of Interest The authors declare no competing interests.

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