Electromagnetic and Thermal nanostructures: from waves to circuits

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Abstract

Nanomaterials have become crucial to develop new technologies in several practical applications fields. Until now nanostructures have been mostly associated with electromagnetism and optics. The aim of this letter is to extend the applicability of such structures also to other wave-based phenomena, such as thermodynamics. Here, in analogy to electric nanocircuits, we present the concept of thermal circuit nanoelements. The basic circuit elements, namely, resistors, capacitors and inductors, are evaluated in terms of electromagnetic (electric permittivity ε) and thermal (conductivity k and convection coefficient h) nanostructure properties. Coupled nanocircuits and parallel/series combinations are also developed. The multi-functional nanostructure can simultaneously control and manipulate both electromagnetic and thermal waves, paving the way to realize more complex electrical and thermal devices.

Keywords: nanostructure, circuit model, electromagnetic wave, conduction, convective.

Electromagnetic nanostructures [1] become well-established technologies in several practical areas: electrical and electronic engineering, life science, computing and telecommunications [2]. In the last decade, theoretical models [3], design methods [4], characterization tools [5], and additive fabrication techniques [6] have been developed to exploit at best their potential. Historically, nanomaterials have been mainly associated with electromagnetism and optics [7]. Only recently, there have been few attempts to apply such concept to other physical domains [8]: the litteratrure on this topic is mostly theoretical [9], and real-life experiments are still in their infancy [10]. The idea is the possibility of using a single structure to simultaneously control and manipulate more than one physical phenomenon.

One of the most important issue in practical devices, is the need for both reliable electrical and thermal management, without affecting the device performances. This is critical to a wide range of industrial applications that enable our modern lives. For this reason, in this letter, we model and design a multi-functional material (nanostructure), able to control at the same time both electrical and thermal phenomena. The aim is to represent both the structure electromagnetic and thermal properties, with its equivalent circuit model. In the electromagnetic domain, structures that are electrically small (dimensions much smaller than the operative wavelength λ) [11], have their electric and magnetic phenomena described by their equivalent lumped elements (R Resistance, C Capacitance and L Inductance). Similarly, in the following we explore how such circuit concepts and elements can be extended to the thermal domain. In the thermal domain, structures that are thermally small (dimensions much smaller than their thermal wavelength λ_{th}) [12], have their conductive and convective phenomena represented by their equivalent circuit elements: R_{th} Thermal Resistance, C_{th} Heat Capacitance and L_{th} Convective Inductance.

Let's consider the simple sphere of Fig.1(a) with radius *r* and homogeneous electromagnetic and thermal properties: electric permittivity ε, magnetic permeability μ, thermal conductivity *k*, and convection coefficient *h*. Immersed in a surrounding environment (homogeneous material) like air, with the following properties: electric permittivity ε_0, magnetic permeability μ_0, thermal conductivity k_0, and convection coefficient h_0.

Consider an incident (electromagentic or thermal) wave illuminating this sphere. It is known that wave equation in homogeneous materials is easily solvable, and its solutions are straightforward for almost all the geometries we can envision [13]. For both the electromagnetic and thermal phenomena, we use the Helmholtz equation:

$$\nabla^2\mathbf{F} + \gamma^2\mathbf{F} = \mathbf{J}_{\mathbf{source}} \quad (1)$$

where the vector **F** can be interpreted as the electric field component **E**, or the temperature **T** for the electromagnetic or heat transfer phenomena, respectively; γ the electromagnetic (*β*) or thermal (*B*) wave-vector; $\mathbf{J}_{\mathbf{source}}$ the electromagnetic or heat density currents impressed by the incident wave.

Because of the small size of the particle (with respect to the related wavelength), the electromagnetic and thermal fields (inside and outside) of the sphere can be obtained by using the quasi-static approach [14]: the electric/thermal sources of the considered problem change sufficiently slowly that the system can be taken to be in equilibrium at all times.

From the electromagnetic side, it means that both electric and magnetic field vectors vary slowly with time, and the Maxwell equations can be considered in their static form (equations that do not involve time derivative) to derive the related equivalent electrical circuit model from the electric/magnetic potential [15].

From the thermal point of view, the quasi-static process happens slowly enough for the system to remain in internal equilibrium: i.e. in the collision-less regime the volume of a system changes at a slow rate enough to allow the pressure to remain uniform and constant throughout the system. Like the electro/magneto -static case, in the thermal-static process we can define lumped quantities (such as thermal resistance) from the related temperature-driven potential of the system [16].

Consequently, the determination of the fields inside and outside the particle can be obtained similarly to [11], extended to the thermal case. From Fig.1(b), the field of the sphere ($\mathbf{F_{int}}$) is a function of the incident field ($\mathbf{F_0}$) as $\mathbf{F_{int}}=\alpha\cdot\mathbf{F_0}$; the external field ($\mathbf{F_{ext}}$) is the superimposition of the incident field ($\mathbf{F_0}$) and the dipolar (electric/temperature-driven) field ($\mathbf{F_{dip}}$) with dipole moment $\boldsymbol{p}=\alpha\cdot\mathbf{F_0}$; and the polarizability α for a generic shape particle is defined as:

$$\alpha = \frac{V\delta_0(\delta_1-\delta_0)}{\delta_0+L(\delta_1-\delta_0)} \quad (2)$$

where *V* is the particle volume; δ_i is either the particle electric permittivity ε_i or the thermal conductivity k_i; *L* the depolarization factor of the particle (for sphere *L*=1/3); with *i*=0, 1, the index for enviroment or particle, respectively.

Thereofore, electric and thermal fields take different expressions according to geometry (sphere), (electromagnetic & thermal) boundary conditions, and materials properties (electric permittivity ε and thermal properties *k*,*h*).

In both electromagnetic and thermal scenarios, at any point on the sphere surface, the normal components of displacement current **D**(α) [15] and heat density current **q**(α) [16] are continuous, Fig.1(b), as:

$$\mathbf{F_0}\cdot\hat{\mathbf{n}} = \mathbf{F_{dip}}\cdot\hat{\mathbf{n}} + \mathbf{F_{res}}\cdot\hat{\mathbf{n}} = \\ = \begin{cases} -j\omega(\varepsilon-\varepsilon_0)\mathbf{E_0}\cdot\hat{\mathbf{n}} = -j\omega\varepsilon_0\mathbf{E_{dip}}\cdot\hat{\mathbf{n}} + j\omega\varepsilon\mathbf{E_{res}}\cdot\hat{\mathbf{n}} \\ \left(\dfrac{1}{k+h}\right)\mathbf{T_0}\cdot\hat{\mathbf{n}} = -kA\cdot\mathbf{T_{dip}}\cdot\hat{\mathbf{n}} + Nu\cdot\mathbf{T_{res}}\cdot\hat{\mathbf{n}} \end{cases} \quad (3)$$

where *A* is the superficial area, *Nu* is the Nusselt defined as Nu= *h*l/*k*, l the physical length of the particle.

We can now relate both field and current densities vectors to their scalar circuit counterparts for both the electromagnetic and thermal wave phenomena. This implies that the total (displacement or heat) current vector can be written as the sum of scalar (electric or heat) currents, named accordingly to their function, in a similar way to what have done in [11] for electromagnetic-only nanostructures: the impressed current source (I_{imp}), the current circulating within the particle (I_{sph}) and the current of the dipolar effect (I_{fringe}), respectively.

Such currents obey for both electric and thermal phenomena, to the Kirchhoff current law, represented by the equations in (3). In addition, also the Kirchhoff voltage law is satisfied, since the curl of the electric and thermal fields ($\nabla\times\mathbf{E}=0, \nabla\times\mathbf{T}=0$) are zero in the quasi-static approximation [17]. The related electric/thermal circuit model is shown in Fig.1(c).

The equivalent electrical/thermal impedances for the sphere and outside branches of the circuit, are calculated as the ratio between the (electric/temperature-driven) potential difference across the upper and lower hemispherical surfaces of the sphere (Fig.1(b)) and the effective currents evaluated from the electromagnetic boundary conditions in (3) (Fig.1(c)). Such impedances (electrically/thermally) behave differently according to the value of the material electric permittivity ε and Nusselt number *Nu*.

- The electromagnetic impedance is based on the sign of the real part of the material permittivity: a *capacitor* or an *inductor*, being positive Re{ε}>0, or negative Re{ε}<0, respectively. The imaginary part, Im{ε}≠0, provides the equivalent resistor.

- The thermal impedance, instead, the Nu number dictates its behavior. Being smaller than unity Nu<1, heat conduction prevails within the medium: we are considering the medium as a solid the heat transfer is exclusively due to conduction. The thermal behavior is capacitive C_{th} taking into account the temperature-driven potential energy stored in the solid particle. The conduction coefficient k determines the thermal resistance R_{th}. The total thermal impedance (**Z₁**) is always a resistor (R_{cond}) in series to a capacitor (C_{cond}), as shown in Fig. 1(d):

$$Z_{in\_sphere} = Z_1 = \begin{cases} R_{cond} = l_c / kA = 1/C_{ele}(\varepsilon \to k) \\ C_{cond} = 1/R_{cond} \end{cases} \quad (4)$$

Like electrical permittivity and magnetic permeability in the electromagnetic realm, thermal coefficients can assume positive or negative values if they are in the form of traditional materials encountered in nature [16], or in a metamaterial-like arrangement [18], respectively.

Outside the sphere, the external environment (electric/thermal) properties assume a crucial role in determining the equivalent (electrical/thermal) circuit model impedance we need to use.

The electromagnetic impedance, outside the particle Z_{fringe} is always capacitive, since we assumed that the permittivity of the outside region (air) is positive ε_0.

Dually for the thermal impedance. The external environment can be solid (particles immersed in a supporting substrate) or fluid (particles immersed in a fluid environment); therefore, the related thermal properties and impedances (**Z₂**) will change accordingly. To this regard, let us consider the following two possible cases:

- If no bulk fluid motion outside the sphere is present (particles immersed in a supporting solid substrate), Nu≤1, therefore the heat flux is obtained by conduction outside the sphere. Since conduction is still present ($q_{out\_sphere}=kS\Delta T$), the outside impedance Z_{out_sphere} is resistive R_{out_sphere} along with its capacitive part C_{out_sphere}, in a similar way to what happened within the sphere:

$$Z_{out\_sphere} = Z_1 = \begin{cases} R_{cond} = 1/(k \cdot S) = 1/C_{ele}(\varepsilon \to k) \\ C_{cond} = \omega(k \cdot S) \end{cases} \quad (5.1)$$

It is worth noting that, since there is only one reactive element (equivalent to a RC electric circuit), there is no resonance present in this case.

- If bulk fluid motion outside of the sphere is considered (particles immersed in a fluid environment), the heat flux is convective (Nu>1) close to the sphere surface. In particular, the heated sphere in the proximity of the fluid creates vortices (convection currents) that possess a kinetic energy. Due to the presence of it, the related heat flow possess inertia: if the temperature difference (driving the convection current) changes, there will be a lag before the heat reaches its steady value. In analogy to the magnetic field and electric current principle across an electrical inductor, the thermal inductance of the fluid is proportional the kinetic energy stored in the convection field in proximity to the sphere surface [19]. The thermal behaviour is inductive L_{conv}, taking into account of the energy stored within the external surrounding fluid in motion [20]. The total thermal impedance outside the sphere (**Z₂**) will be interpreted as a resistance in series with an inductance, as shown in Fig. 1(d):

$$Z_{out\_sphere} = Z_2 = \begin{cases} R_{conv} = l_c/(hA_s) \\ L_{conv} = \omega(1/R_{conv}) = \omega(1/C_{ele}(\varepsilon \to h)) \end{cases} \quad (5.2)$$

In this case, since there is a reactive element (an inductor) in parallel to the particle reactive element (RC circuit), the circuit may exhibit thermal resonance, which corresponds to the electromagnetic resonance in the equivalent electric circuits of the same particle.

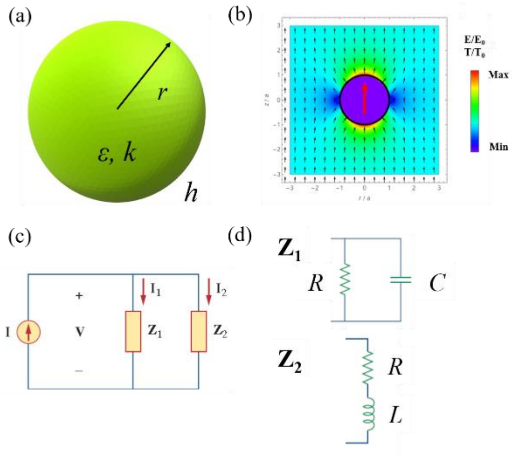

Fig.1: (a) Nanosphere structure of radius r: silver particles (with radius in the range 50-100 nm), electric permittivity $\varepsilon_{Ag} = (-19 + j0.53)\varepsilon_0$ [11], thermal conductivity k=429 W/m·K; external environment (air) with thermal conductivity k_{air}= 0.026 W/m·K and convection coefficient h in the range of 10 – 30 W/m^2·K. (b) Electric/Thermal field distribution across the nanosphere: solid red arrow show the incident electric/thermal field; thinner field arrows represent the fringe dipolar electric/thermal field from the sphere. (c) Equivalent electric/thermal circuit model: **Z₁** total electric/thermal particle impedance, **Z₂** total electric/thermal external impedance (d) Details for the impedances Z_1 and Z_2 of the circuit in (c): parallel resistor-capacitor, and series resistor-inductor.

It follows from the above discussion that we can always represent a material in terms of electromagnetic and thermic phenomena, by using their equivalent (electric/thermal) circuit model. In this letter, a small sphere excited by an external (electromagnetic/thermal) signal may effectively behave as a (electric/thermal) capacitor or inductor, as a function of the permittivity (real part) value or Nu number, for the electromagnetic or thermal case, respectively. The resistor is determined by the imaginary part of the permittivity or the thermal conduction/convective coefficients value of the material for the electromagnetic or thermal case, respectively. The value of each circuit element can be designed by properly selecting the size, shape, and material contents of the structure. Table 2 summarises the resistor, capacitor and inductor values for both electrical and thermal elements of the sphere. It is worth noting that since the thermal circuit behaviour is dual to its electrical counterpart, even its elements will be dual. In other words, starting from the well-known and established electric circuit, we can evaluate in a straightforward manner the related thermal circuit, and vice-versa. These concepts provide new possibilities for both structure miniaturization and the simultaneous control of both electromagnetic (permittivity ε) and thermal (k, h) properties, in different frequency ranges.

TABLE 2: RESISTOR, CAPACITOR AND INDUCTOR ELECTRIC AND THERMAL VALUES .

	Electric circuit [11]	**Thermal circuit**
Resistor	$G_{ele}=\pi\omega r\mathrm{Im}[\varepsilon]$	$R_{in\_sphere}=\frac{1}{C_{sph}(\varepsilon\rightarrow k)}$ $R_{out\_sphere}=\begin{cases} R_{cond}=R_{in\_sphere} \\ R_{conv}=\frac{1}{C_{sph}(\varepsilon\rightarrow h)} \end{cases}$
Capacitor	$C_{sph}= 4\pi r\mathrm{Re}[\varepsilon]$ $C_{fringe}= 2\pi\omega r\varepsilon_0$	$C_{in\_sphere}=\frac{1}{R_{in\_sphere}(k\rightarrow \rho c_p)}$ $C_{out\_sphere}=C_{in\_sphere}$
Inductor	$L_{ele}= (-\omega^2\pi r\mathrm{Re}[\varepsilon])^{-1}$	$L_{conv}=\omega\frac{1}{C_{fringe}(\varepsilon\rightarrow h)}$

The three basic electric and thermal circuit elements (Resistor, Capacitor and Inductor) previously obtained, form the building blocks for the design of more complex circuits. To this regard, we can expand this concept to configurations with more than one nanoparticle: the case of two spheres (Fig.2(a)) with different radii r_1 and r_2, permittivity ε_1 and ε_2, thermal parameters (k_1, h_1) and (k_2, h_2) and with a certain distance d apart. Both electromagnetic and thermal (Fig.2(b)) analysis of the fields distribution shows that such configurations can be treated as electrically and thermally coupled circuits, each representing one of the spheres.

Therefore, in addition to the elements depicted in Fig. 1 for the isolated sphere, in the case of coupled spheres each circuit should also include a dependent current I (voltage V) source [16], in parallel (series) with an equivalent admittance Y_{eq} (impedance Z_{eq}), as shown in Fig.2(c). This circuit will represent the influence of the electric/temperature field of the other particle on the considered sphere.

For both cases (electromagnetic and thermal), the value of each dependent source is function of the (induced electric/driven temperature) potential difference across the other particle. On the other hand, the evaluation of the equivalent impedance $Z_{coupling}$ will depend on two elements:

(*i*) The electric and thermal circuit elements in the circuit of the other particle. Therefore, for the electric case, such value will depend on the capacitive or inductive nature of the other sphere. For the thermal case, $Z_{coupling}$ will depend on the heat transfer method within the other sphere and outside the spheres (presence or not of fluid motion).

(*ii*) Any electric or thermal coupling across the two particles. For the former mutual capacitance or inductance, for the latter thermal conduction or convection [17].

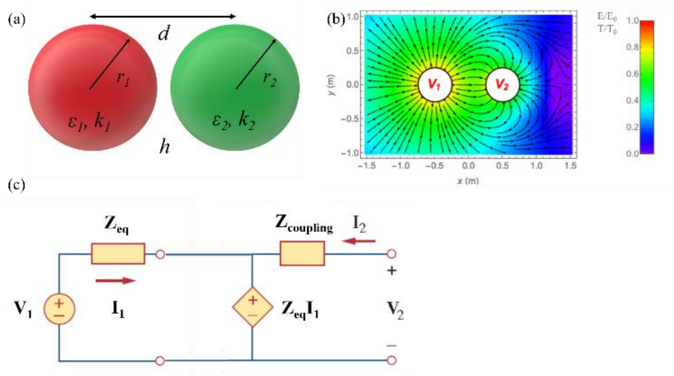

Fig.2: (a) Couple nanospheres of radius r_1 and r_2, with electric and thermal properties (ε_1,k_1) and (ε_2,k_2), respectively, distances in the range of 50-100 nm; (b) Electric/Thermal field distribution across the coupled nanospheres; (c) Equivalent electric/thermal circuit model for the nanospheres shown in (a).

In order to form parallel and/or series circuit elements with these particles [21], in both cases we can juxtapose two (or more) materials very closely with specific electric/thermal parameters and orientation with respect to the impinging electric/temperature field. Fig.3(a) shows the geometry of two paired semi-spheres of differing electric permittivity and thermal parameters. The distribution of electric and temperature potential (Fig.3(b)) around the new merged structure, is crucial to understand the combined circuit elements behaviour.

In the cases of electric and temperature field being parallel to the plane interface between the two halves, the combined structure is a *parallel* (resonant) circuit [22]. This is because the electric and temperature field lines are perpendicular to the outer particle surface, implying that there is indeed a certain potential difference between the top and bottom parts of the sphere's surface (Z_1). In addition to this, we need also to consider (Z_2) both (*i*) the electric potential drop across the interface due to contact phenomena of two different materials (electric conductance or contact capacitance); and (*ii*) the temperature drop at the interface due to the non-perfect contact of the two layers (thermal contact conductance). Finally, the total circuit will be in parallel with the outside the sphere impedance Z_N (electric fringe capacitor, thermal resistance/inductor).

The equivalent electric/thermal circuit model is reported in Fig. 3(c). Fig.3(d), showing the lumped circuit elements in detail. Dual behaviour (electrical and thermal) if the electric and temperature fields are perpendicular to the boundary interface between the two hemi-spheres: the circuit is a *series* (resonant) circuit. Even in this case the resonant behaviour is present due to the particular choice of oppositely signed for the permittivity and small/great values of Nu.

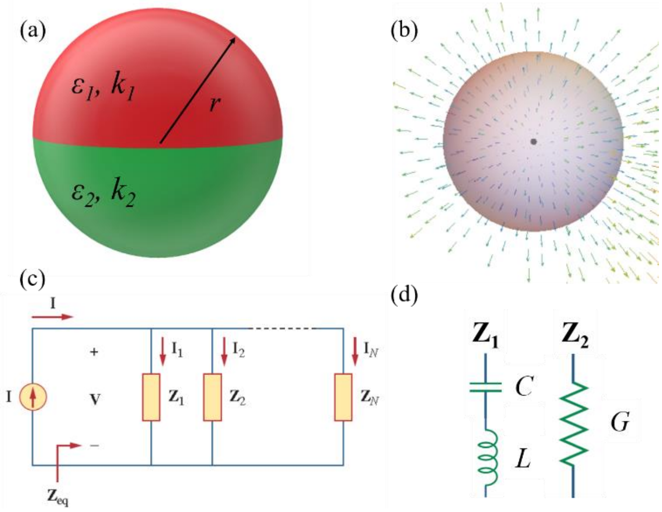

Fig.3: (a) Nanoparticle structure obtained by fusing two hemi-spherical particles of same radius *r*, with different electric and thermal properties (ε_1,k_1) and (ε_2,k_2), respectively; (b) Distribution of electric/temperature potential across the new nanosphere; (c) Equivalent electric/thermal circuit model for the fused structure; (d) Details of the impedances $\mathbf{Z_1}$ and $\mathbf{Z_2}$ of the circuit in (c). Z_N can be either $\mathbf{Z_1}$ or $\mathbf{Z_2}$ of Fig.1(d), if fluid motion is present or not, respectively.

Finally, it should be point out that by properly arranging these nanoscale circuit elements it is possible to create electromagnetic and thermal transmission-lines. Like in the domain of electromagnetic structures, even in the thermal realm if the arrangement involves series of inductors and shunt capacitors, for the dominant even mode this will provide conventional uniform transmission lines, similarly to what has been proposed in [23] for the electrical case. However, if shunt inductors and series capacitors are implemented, we synthesize left-handed transmission lines, similarly to what was proposed for electromagnetic metamaterials [24].

In this letter, a new circuit modelling approach had been proposed for arbitrary shape nanostructures. Such a model permits to obtain full control of the nanostructure electromagnetic and thermal properties. By using the proposed electric/thermal circuit model, we can manipulate at will the nanoparticle features according to the required application. Such circuits, in fact, can find applications in different fields such as sensing; subwavelength optical imaging and thermal focusing effects for medical diagnostics; or advanced data storage systems.

The multi-factional nanostructure concept, with the appropriate corrections and analogies, can be extended to other wave-based phenomena such as acoustics, fluid dynamics and classical mechanics. Future and undergoing works are based on the exploration of such concepts.

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