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Research Article

A Nonlocal Model for Carbon Nanotubes under Axial Loads

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Various beam theories are formulated in literature using the nonlocal differential constitutive relation proposed by Eringen. A new variational framework is derived in the present paper by following a consistent thermodynamic approach based on a nonlocal constitutive law of gradient-type. Contrary to the results obtained by Eringen, the new model exhibits the nonlocality effect also for constant axial load distributions. The treatment can be adopted to get new benchmarks for numerical analyses.

1. Introduction

Carbon nanotubes (CNTs) are a topic of major interest both from theoretical and applicative points of view. This subject is widely investigated in literature to describe small-scale effects [1–4], vibration and buckling [5–13], and nonlocal finite element analysis [14–18]. A comprehensive review on applications of nonlocal elastic models for CNTs is reported in [19] and therein references. Buckling of triple-walled CNTs under temperature fields is dealt with in [20]. An alternative methodology is based on an atomistic-based approach [21] which predicts the positions of atoms in terms of interactive forces and boundary conditions. The standard approach to analyze CNTs under axial loads consists in solving an inhomogeneous second-order ordinary differential equation providing the axial displacement field, see, for example, [22]. The known term of the differential equation is the sum of two contributions. The former describes the local effects linearly depending on the axial load. The latter characterizes the small-scale effects depending linearly on the second derivative along the rod axis of the axial load. This model is thus not able to evaluate small-scale effects due to, constant axial loads per unit length. This approach, commonly adopted in literature, is based on the following nonlocal linearly elastic constitutive law proposed by Eringen [23]:

$$\sigma - e_o^2 a^2 \sigma^{(2)} = E\varepsilon, \tag{1}$$

where e_o is a material constant, a is the internal length, E is the Young modulus, σ is the normal stress, the apex $(\bullet)^{(2)}$ is second derivative along the rod axis, and ε is the axial elongation. Indeed, integrating on the rod cross section domain Ω and imposing that the axial force N is equal to the resultant of normal stress field we get the differential equation

$$N - e_o^2 a^2 N^{(2)} = EAw^{(1)}, \tag{2}$$

where $\varepsilon = w^{(1)}$, with $w^{(1)}$ being first derivative along the rod axis of the axial displacement field $w : [0, L] \mapsto \mathcal{R}$, where L is the rod length and A denotes the cross section area. Since the equilibrium prescribes that the first derivative of N is opposite to the axial load p, we infer the well-known differential equation (see, e.g., [7]) as follows:

$$w^{(2)} = \frac{-p + e_o^2 a^2 p^{(2)}}{EA}. \tag{3}$$

Note that the nonlocal contribution vanishes for constant loads p. In the present paper, an alternative nonlocal constitutive behavior is adopted to assess small-scale effects in nanotubes also for constant axial loads. The corresponding axial displacement field is shown to be governed by a fourth-order inhomogeneous differential equation. Boundary conditions are naturally inferred by performing a standard localization procedure of a variational problem formulated by making recourse to thermodynamic restrictions see, for example, [24–26], according to the geometric approach illustrated in [27–30]. As an example, the displacement field of nanotubes under constant axial loads per unit length is evaluated in the appendix. Vibration and buckling effects are not the subject of this paper and will be addressed in a forthcoming paper.

2. Nonlocal Variational Formulation

Let $\mathscr{B}$ be the three-dimensional spatial domain of a straight rod subjected to axial loads. An apex $(\bullet)^{(n)}$ stands for nth derivative along the rod centroidal z-axis. Kinematic compatibility between axial elongations ε and axial displacements w is expressed by the differential equation $\varepsilon = w^{(1)}$. Denoting by a dot the time-rate, the following noteworthy relations hold true

$$\dot{\varepsilon} = \dot{w}^{(1)}, \qquad \dot{\varepsilon}^{(1)} = \dot{w}^{(2)}. \tag{4}$$

The differential equation of equilibrium turns out to be $N^{(1)} = -p$. Boundary equilibrium prescribes that at the end cross sections act axial loads equal to $N(0)$ for $z = 0$ and to $N(L)$ for $z = L$. Let us now consider a nonlocal constitutive model of gradient-type defined by assigning the following elastic energy functional per unit volume:

$$\psi\left(\varepsilon, \varepsilon^{(1)}\right) := \frac{1}{2}E\varepsilon^2 + \frac{1}{2}Ec^2\varepsilon^{(1)^2}, \tag{5}$$

with $c := e_o a$ being nonlocal parameter. Relation (5) is similar to the elastic energy density proposed in [31] where a homogeneous quadratic functional including also mixed terms is assumed. The elastic energy time rate is hence expressed by the formula

$$\dot{\psi}\left(\varepsilon, \varepsilon^{(1)}\right) = \frac{\partial\psi}{\partial\varepsilon}\dot{\varepsilon} + \frac{\partial\psi}{\partial\varepsilon^{(1)}}\dot{\varepsilon}^{(1)} = \sigma_o\dot{\varepsilon} + \sigma_1\dot{\varepsilon}^{(1)}, \tag{6}$$

where

$$\sigma_o := \frac{\partial\psi}{\partial\varepsilon} = E\varepsilon, \qquad \sigma_1 := \frac{\partial\psi}{\partial\varepsilon^{(1)}} = Ec^2\varepsilon^{(1)}, \tag{7}$$

are the static variables conjugating with the kinematic variables ε and $\varepsilon^{(1)}$. The static variable σ_1 is the scalar counterpart of the so-called double stress tensor [31]. By imposing the thermodynamic condition (see, e.g., [32–34])

$$\int_{\mathscr{B}} \sigma\, \dot{\varepsilon} dV - \int_{\mathscr{B}} \dot{\psi} dV = 0, \tag{8}$$

where σ is the normal stress, we infer the relation

$$\int_{\mathscr{B}} \sigma\dot{\varepsilon} dV = \int_{\mathscr{B}} \sigma_o\dot{\varepsilon} dV + \int_{\mathscr{B}} \sigma_1\dot{\varepsilon}^{(1)} dV. \tag{9}$$

The relevant differential and boundary equations are thus obtained as shown hereafter. Substituting the expression of the rates $\dot{\varepsilon}$ and $\dot{\varepsilon}^{(1)}$ in terms of the axial displacement $w(z)$ of the cross section at abscissa z, we get the formulae

$$\begin{aligned}
\int_{\mathscr{B}} \sigma\dot{\varepsilon} dV &= \int_{\mathscr{B}} \sigma\dot{w}^{(1)} dV = \int_0^L \left(\int_\Omega \sigma dA\right)\dot{w}^{(1)} dz \\
&= \int_0^L N\dot{w}^{(1)} dz, \\
\int_{\mathscr{B}} \sigma_o\dot{\varepsilon} dV &= \int_0^L N_o\dot{w}^{(1)} dz, \\
\int_{\mathscr{B}} \sigma_1\dot{\varepsilon}^{(1)} dV &= \int_{\mathscr{B}} \sigma_1\dot{w}^{(2)} dV = \int_0^L \left(\int_\Omega \sigma_1\, dA\right)\dot{w}^{(2)} dz \\
&= \int_0^L N_1\dot{w}^{(2)} dz,
\end{aligned} \tag{10}$$

with $N = \int_\Omega \sigma dA$ axial force (static equivalence condition on the cross sections) and $N_i := \int_\Omega \sigma_i dA$ for $i \in \{0, 1\}$. Thermodynamic condition (9) provides the axial contribution

$$\int_0^L N\dot{w}^{(1)} dz = \int_0^L N_o\dot{w}^{(1)} dz + \int_0^L N_1\dot{w}^{(2)} dz. \tag{11}$$

3. Differential and Boundary Equations of Elastic Equilibrium

Resorting to Green's formula, a standard localization procedure provides the differential and boundary equations corresponding to the variational conditions inferred in Section 2, as follows. A direct computation gives

$$\begin{aligned}
\int_0^L N\dot{w}^{(1)} dz &= [N\ \dot{w}]_0^L - \int_0^L N^{(1)}\dot{w} dz, \\
\int_0^L N_o\dot{w}^{(1)} dz &= [N_o\ \dot{w}]_0^L - \int_0^L N_o^{(1)}\dot{w} dz, \\
\int_0^L N_1\dot{w}^{(2)} dz &= \left[N_1\ \dot{w}^{(1)}\right]_0^L - \int_0^L N_1^{(1)}\dot{w}^{(1)} dz \\
&= \left[N_1\ \dot{w}^{(1)}\right]_0^L - \left[N_1^{(1)}\ \dot{w}\right]_0^L + \int_0^L N_1^{(2)}\dot{w} dz.
\end{aligned} \tag{12}$$

Substituting into the variational condition (11), a suitable localization provides the relevant differential equation

$$N^{(1)} = N_o^{(1)} - N_1^{(2)} \tag{13}$$

and boundary conditions

$$\begin{aligned}
N &= N_o - N_1^{(1)}, \quad \text{dual of } \dot{w}, \\
0 &= N_1, \quad \text{dual of } \dot{w}^{(1)}.
\end{aligned} \tag{14}$$

These conditions can be conveniently expressed in terms of the axial displacement field w as follows. A direct evaluation of the scalar functions $N_i : [0, L] \mapsto \mathscr{R}$ for $i \in \{0, 1\}$ and of their derivatives gives

$$\begin{gathered} N_o = \int_\Omega \sigma_o dA = \int_\Omega E\varepsilon dA = \int_\Omega E w^{(1)} dA = EAw^{(1)}, \\ N_o^{(j)} = EAw^{(1+j)}, \\ N_1 = \int_\Omega \sigma_1 dA = \int_\Omega E c^2 \varepsilon^{(1)} dA \\ = \int_\Omega E c^2 w^{(2)} dA = EAc^2 w^{(2)}, \\ N_1^{(j)} = EAc^2 w^{(2+j)}, \end{gathered} \tag{15}$$

with $j \in \{1, 2, \ldots, n\}$. Accordingly, the boundary and differential conditions of elastic equilibrium (13) and (14) take the form

$$\begin{gathered} N^{(1)} = N_o^{(1)} - N_1^{(2)} = EAw^{(2)} - EAc^2 w^{(4)}, \\ N = N_o - N_1^{(1)} = EAw^{(1)} - EAc^2 w^{(3)}, \quad \text{dual of } \dot{w}, \\ 0 = N_1 = E\ A\ c^2 w^{(2)}, \quad \text{dual of } \dot{w}^{(1)}. \end{gathered} \tag{16}$$

4. Example

Let us consider a straight rod subject to a constant axial load p as depicted in Figure 1. End cross sections **A** and **B** are assumed to be hinged and simply supported, respectively. As illustrated in Section 3, the computation of the rod axial displacement field w involves the following cross section geometric and elastic properties: area A, Young modulus E, and nonlocal parameter c. By setting $\alpha := EAc^2$ and $\beta := EA$, the differential equation of elastic equilibrium is as follows:

$$\alpha w^{(4)} - \beta w^{(2)} = p. \tag{17}$$

The general integral takes thus the form (see the appendix)

$$w(z) = w_H(z) + \overline{w}(z), \tag{18}$$

with

$$\begin{gathered} w_H(z) = c_1 + c_2 z + c_3 \exp\left(\sqrt{\frac{\beta}{\alpha}} z\right) \\ + c_4 \exp\left(-\sqrt{\frac{\beta}{\alpha}} z\right), \\ \overline{w}(z) = c_5 z^2. \end{gathered} \tag{19}$$

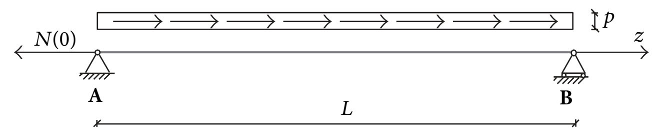

Figure 1: Rod under constant axial load.

The evaluation of the constants is carried out by imposing the following boundary conditions (see also Section 3):

$$\begin{gathered} w(0) = 0, \\ N(L) = EAw^{(1)}(L) - EAc^2 w^{(3)}(L) = 0, \\ N_1(0) = EAc^2 w^{(2)}(0) = 0, \\ N_1(L) = EAc^2 w^{(2)}(L) = 0, \\ \Updownarrow \\ w(0) = 0, \\ w^{(1)}(L) - c^2 w^{(3)}(L) = 0, \\ w^{(2)}(0) = 0, \\ w^{(2)}(L) = 0. \end{gathered} \tag{20}$$

Resorting to the expressions of the derivatives $w_H^{(j)}$ and $\overline{w}^{(j)}$ for $j \in \{1, 2, 3, 4\}$,

$$\begin{gathered} w_H^{(1)}(z) = c_2 + \frac{c_3}{c} \exp\left(\frac{1}{c} z\right) - \frac{c_4}{c} \exp\left(-\frac{1}{c} z\right), \\ w_H^{(2)}(z) = \frac{c_3}{c^2} \exp\left(\frac{1}{c} z\right) + \frac{c_4}{c^2} \exp\left(-\frac{1}{c} z\right), \\ w_H^{(3)}(z) = \frac{c_3}{c^3} \exp\left(\frac{1}{c} z\right) - \frac{c_4}{c^3} \exp\left(-\frac{1}{c} z\right), \\ w_H^{(4)}(z) = \frac{c_3}{c^4} \exp\left(\frac{1}{c} z\right) + \frac{c_4}{c^4} \exp\left(-\frac{1}{c} z\right), \\ \overline{w}^{(1)}(z) = 2c_5 z, \\ \overline{w}^{(2)}(z) = 2c_5, \\ \overline{w}^{(3)}(z) = 0, \\ \overline{w}^{(4)}(z) = 0, \end{gathered} \tag{21}$$

and having $\sqrt{\beta/\alpha} = 1/c$, a direct computation provides the algebraic system

$$\begin{gathered} c_1 + c_3 + c_4 = 0, \\ c_2 + 2Lc_5 = 0, \\ \frac{1}{c^2} c_3 + \frac{1}{c^2} c_4 + 2c_5 = 0, \\ \frac{1}{c^2} \exp\left(\frac{1}{c} L\right) c_3 + \frac{1}{c^2} \exp\left(-\frac{1}{c} L\right) c_4 + 2c_5 = 0. \end{gathered} \tag{22}$$

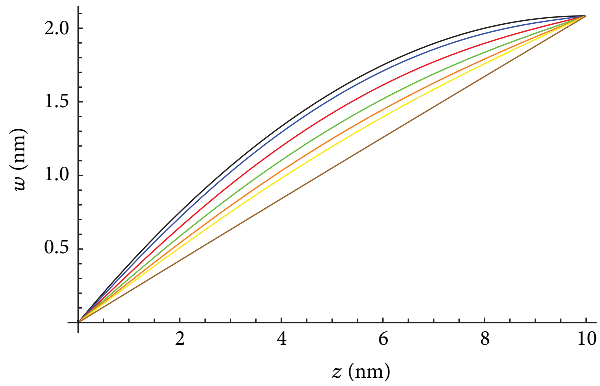

FIGURE 2: Axial displacement field w for $c = 0$ (local solution—black line), $c = 1$ nm (blue line), $c = 2$ nm (red line), $c = 3$ nm (green line), $c = 4$ nm (orange line), $c = 5$ nm (yellow line), and $c = 25$ nm (brown line). $E = 300$ GPa; $L = 10$ nm; $A = 80 \cdot 10^{-2}$ nm^2; and $p = 10^{-8}$ N/nm.

A further condition can be obtained by imposing that the scalar field

$$\overline{w}(z) = c_5 z^2 \tag{23}$$

is a particular solution of the differential equation (17), whence it follows that $c_5 = -p/2EA$. The remaining constants are given by the formulae

$$\begin{aligned} c_1 &= -(c_3 + c_4), \\ c_2 &= -2Lc_5, \\ c_3 &= \frac{2c^2(1 - \exp(-(1/c)L))}{\exp(-(1/c)L) - \exp((1/c)L)} c_5, \\ c_4 &= \frac{2c^2(1 - \exp((1/c)L))}{\exp((1/c)L) - \exp(-(1/c)L)} c_5, \end{aligned} \tag{24}$$

having $c_5 = -p/2EA$. A plot of the rod axial displacement field w for different values of the nonlocal parameter c is provided in Figure 2. It is apparent that the rod becomes stiffer if the nonlocal parameter increases. The evaluated axial displacement at the free end of the rod **B** provides the same value independently of the nonlocal parameter. Such a value coincides with the displacement of the point **B** if a local model is considered. Moreover, the limit of the axial displacement field for c tending to plus infinity can be evaluated to get the lower bound

$$w^{\text{low}}(z) := \lim_{c \to +\infty} w(z, c) = 0.208333z. \tag{25}$$

Hence, large values of the nonlocal parameter provide a displacement field which tends to a linear one, see Figure 2, for $c = 25$. Further, the limit value of the axial displacement for $z = L$ and $c \to +\infty$, obtained by (25), yields $w^{\text{low}}(L) =$ 2.08333 nm which coincides with the axial displacement at **B** for any value of the nonlocal parameter c, see Figure 3 and Table 1.

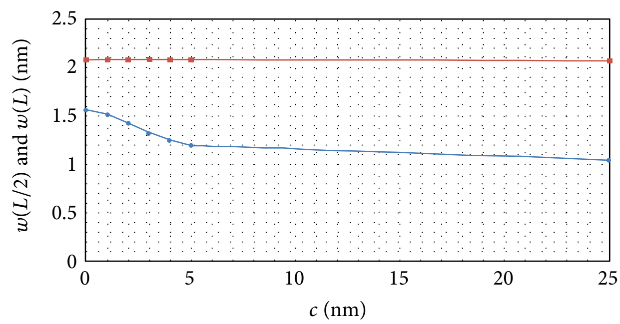

FIGURE 3: Axial displacement in terms of the nonlocal parameter c at the abscissa $z = L/2$ (blue line) and $z = L$ (red line).

TABLE 1: Axial displacements $w(L/2)$ and $w(L)$ versus the nonlocal parameter c.

c (nm)	$w(L/2)$ (nm)	$w(L)$ (nm)
0	1.5625	2.08333
1	1.52139	2.08333
2	1.42301	2.08333
3	1.32428	2.08333
4	1.24886	2.08333
5	1.19589	2.08333
25	1.05021	2.08333

The upper bound of the axial displacement is provided by the local solution (i.e., $c = 0$)

$$w^{\text{upp}}(z) := w(z, 0) = \frac{p(z)(2L - z)z}{2EA}. \tag{26}$$

The axial displacement evaluated for $z = L$ by (26) yields the value $w^{\text{upp}}(L) = 25/12$ nm which coincides with the axial displacement at **B** for any value of c, see Figure 3 and Table 1. For the considered model, the upper and lower bounds of the axial displacement field are given by (25) and (26). The axial displacement $w(L/2)$ at the middle point of the rod and the maximum axial displacement $w(L)$ as functions of the nonlocal parameter c are depicted in Figure 3. The corresponding numerical values of $w(L/2)$ and $w(L)$ are listed in Table 1.

It is worth noting that equilibrium prescribes that axial force N must be a linear function, confirmed by the blue diagram in Figure 4 obtained as difference between the local contribution N_o (dashed line) and the nonlocal one $N_1^{(1)}$ (continuous thin line), according to $(14)_1$ for any value of c.

5. Conclusions

The outcomes of the present paper may be summarized as follows.

(i) Linearly elastic carbon nanotubes under axial loads have been investigated by a nonlocal variational approach based on thermodynamic restrictions. The treatment provides an effective tool to evaluate small-scale effects in nanotubes subject also to constant

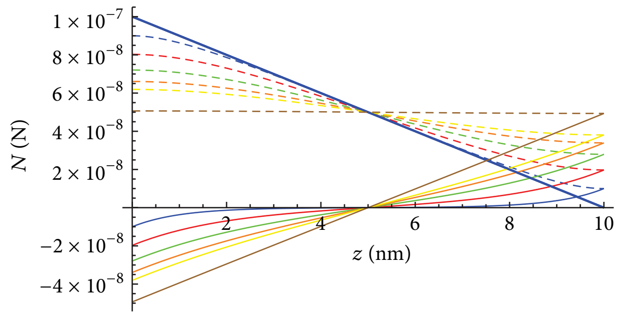

FIGURE 4: Axial force $N = N_o - N_1^{(1)}$ (blue line), N_o (dashed line), $N_1^{(1)}$ (continuous thin line); $c = 0$ (local solution-black line), $c = 1$ nm (blue line), $c = 2$ nm (red line), $c = 3$ nm (green line), $c = 4$ nm (orange line), $c = 5$ nm (yellow line), and $c = 25$ nm (brown line).

axial loads, a goal not achievable by the Eringen model commonly adopted in literature as motivated in Section 1.

(ii) Relevant boundary and differential conditions of elastic equilibrium have been inferred by a standard localization procedure. Such a procedure provides, in a consistent way, the relevant class of boundary conditions for the nonlocal model.

(iii) The present approach yields a firm thermodynamic procedure to derive different nonlocal models for CNTs by suitable specializations of the elastic energy.

(iv) Exact solutions of carbon nanotubes subject to a constant axial load have been obtained. An advantage of the proposed procedure consists in providing an effective tool to be used as a benchmark for numerical analyses. Finally, a range to which any nonlocal solution must belong is analytically evaluated.

Appendix

The procedure to solve the ordinary differential equation

$$\alpha w^{(4)} - \beta w^{(2)} = f, \tag{A.1}$$

with $\alpha, \beta > 0$ being constant coefficients and $f : I \subseteq \mathcal{R} \mapsto \mathcal{R}$ being a continuous function, is summarized as follows. Let us consider the homogeneous differential equation

$$\alpha w^{(4)} - \beta w^{(2)} = 0 \tag{A.2}$$

and the relevant characteristic (algebraic) equation $\alpha\lambda^4 - \beta\lambda^2 = 0$. The roots of the polynomial $\alpha\lambda^4 - \beta\lambda^2$ are $\lambda_1 = 0$ with multiplicity 2, $\lambda_2 = \sqrt{\beta/\alpha}$ with multiplicity 1 and $\lambda_3 = -\sqrt{\beta/\alpha}$ with multiplicity 1. The general integral of (A.2) is thus expressed by the formula

$$w_H(z) = c_1 + c_2 z + c_3 \exp\left(\sqrt{\frac{\beta}{\alpha}}\, z\right) + c_4 \exp\left(-\sqrt{\frac{\beta}{\alpha}}\, z\right), \tag{A.3}$$

with exp denoting exponential function and $c_i \in \mathcal{R}$ for $i = \{1, \ldots, 4\}$. The general integral of (A.1) is writen therefore as

$$w(z) = w_H(z) + \overline{w}(z), \tag{A.4}$$

where $\overline{w}$ is a particular solution of (A.1). It is worth noting that, for f defined by a polynomial p_m of degree $m \geq 0$, the solution $\overline{v}$ can be looked for by setting

$$\overline{w}(z) = z^2\left(A_0 + A_1 z + \cdots + A_m z^m\right), \tag{A.5}$$

with $A_i \in \mathcal{R}$ for $i = \{1, \ldots, m\}$.

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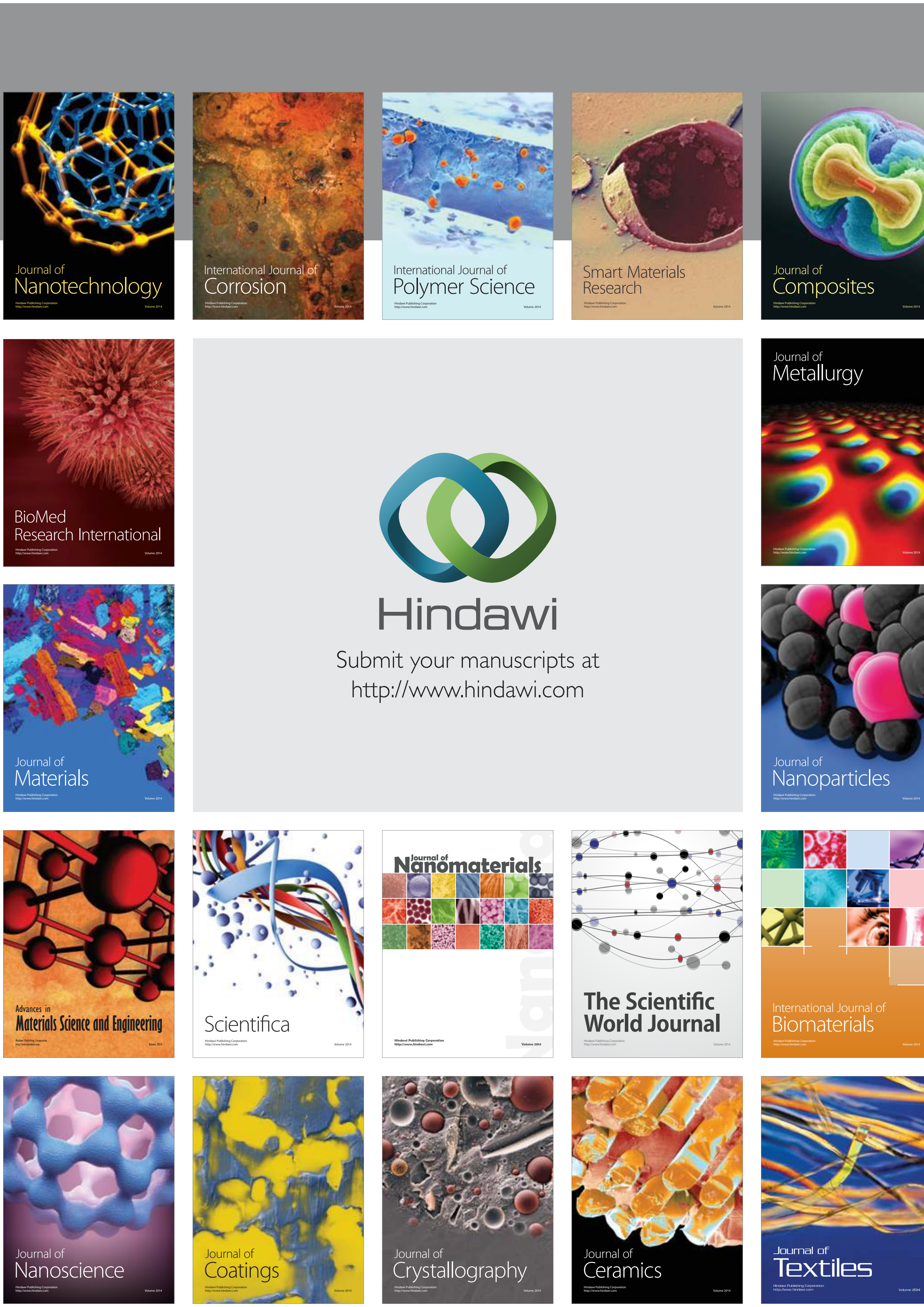

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