

Analytical and numerical study of thermal stresses and stress intensity factors in a concrete nanocomposite with nano-SiO₂ under monotonically increasing temperature

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The analytical and numerical modelling of the behavior of a concrete nanocomposite under monotonically increasing temperature is presented. The research methodology includes analytical modelling based on linear elastic fracture mechanics (LEFM) to determine the thermal stresses and stress intensity factors (SIF) in a concrete nanocomposite with a symmetrically located central crack, considering the influence of both crack length and the temperature. The numerical solutions are obtained by using the specialized software product Wolfram Mathematica, including the generation of special macros to automate the calculations of the thermal stresses and temperature distribution in uncracked and cracked concrete composites, with or without the addition of nanoparticles. The obtained results show that for small cracks, the difference between the SIF values of the two materials (concrete composite without/with 2% nano-SiO₂) is minimal, while for larger cracks the SIF value of the nanocomposite is significantly higher, but not too large, which preserves the relative stability of the material. For example, at a crack length of 0.01 m, the SIF increases from 25.39 MPa·m^{1/2} (without nanoparticles) to 27.55 MPa·m^{1/2} (with nano-SiO₂), illustrating enhanced crack resistance. At the same time, total thermal stresses increase with temperature, reaching values of up to 12.8 MPa in nano-SiO₂ concrete compared to 10.9 MPa in standard concrete at $\Delta T = 100$ °C. The developed mathematical models provide a convenient tool for thermal and fracture analysis, which can be applied in the design of sustainable, durable, and thermally resistant concrete structures.

Keywords: Concrete nanocomposite, nano-SiO₂, central crack, SIF, analytical and numerical results, thermal stresses

INTRODUCTION

Motivation and significance of the study

Concrete is a basic construction material, but its resistance to thermal loads is limited due to its low tensile strength and its tendency to crack at high temperatures [1-3]. The addition of nano-SiO₂ significantly improves the mechanical and thermal properties of concrete by reducing porosity and increasing its thermal stability. Analytical modelling based on linear elastic fracture mechanics (LEFM) and numerical solutions obtained using the finite difference method (FDM) and finite element method (FEM) in Wolfram Mathematica software will be useful for more accurate determination of local and total thermal stresses and SIF values in a concrete nanocomposite with a central crack.

Literature review

Concrete nanocomposites are an innovative class of energy-efficient materials that are gaining increasing popularity in the construction industry due to their exceptional properties and environmental benefits. They combine traditional concrete with nanoparticles, leading to improved mechanical and

thermal properties [4]. Nano-SiO₂ is one of the most effective nano-additives that: change the microstructure of concrete – it reduces porosity and improves bonding between cement paste and aggregates; accelerates cement hydration - leads to faster hardening and increased strength; increases concrete resistance to cracking - increases tensile strength and compressive strength; improves thermal resistance - reduces thermal expansion and increases resistance to temperature loads [5, 6]. The greater strength of concrete with nano-SiO₂ allows for the construction of thinner and lighter structures, which reduces the use of raw materials and leads to lower energy consumption during construction. Concrete nanocomposites with nano-SiO₂ are key materials for sustainable construction, as on the one hand they help reduce the carbon footprint and energy consumption, and on the other hand they increase the durability of buildings and structures [7-11].

During the operation of concrete structures, they are often subjected to temperature effects that can induce thermal stresses and accelerate the development of cracks in them. Understanding the influence of temperature, mechanical and thermo-mechanical loads on stresses and strains, stress

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intensity factors (SIF) and energy release rate (ERR) are essential for assessing the durability and reliability of concrete and other types of nanocomposites [12-23]. The classic work [13] investigates the stress concentration around crack tips using fracture mechanics methods such as stress intensity factor, energy approaches and fracture models to predict the resistance of materials to cracking. The works [14] and [15] analyze the stress distribution at the base of a fixed crack using different theoretical models for stress concentration estimation, critically reviewing existing crack propagation laws, and comparing different criteria for crack growth and resistance. The work [16] presents various analytical and numerical methods for studying crack problems, focusing on fracture mechanics, stresses around cracks and criteria for their propagation. The book [17] is related to fracture mechanics and describes the main guidelines for the analysis of stress concentration in cracks and their propagation. In [18] and [19], detailed formulas and examples for calculating SIF and the influence of various stresses, including temperature stresses, on cracks in materials are proposed. The book [19] also discusses the basic principles of fracture mechanics. In several publications, research has focused on estimating SIF and the rate of energy release for various composite materials, but there is a lack of sufficient data on the behavior of concrete nanocomposites with nano-SiO₂ under temperature effects, [2, 3, 12, 20], etc.

The aim of this study is to supplement the available literature in this area by developing a complex analytical model that covers:

- Calculation of thermal stresses in a concrete composite with/without added 2% of nano-SiO₂ at monotonically increasing temperature.
- Determination of stress intensity factors at different lengths of the initial crack and at different temperature values.
- Analysis of the influence of added nanoparticles in concrete on the values of thermal stress and SIF.

PROBLEM FORMULATION

The concrete nanocomposite is modelled as a rectangular plate with width $2W$, length $2L$ and a central symmetric crack with length $2a$, Figure 1. The plate is subjected to a monotonically increasing temperature with a temperature difference $\Delta T = T_{high} - T_{low}$, where T_{high} and T_{low} are the temperatures of the upper and lower boundaries of the plate, respectively. The direction of the temperature gradient is also shown, namely from the upper to the lower surface. The center of the coordinate system

Oxy , used in the model, is in the middle of the crack. The x -axis is oriented horizontally (along the thickness of the plate) and is symmetric with respect to the crack, i.e., $x \in (-W, W)$. This axis measures the distances to the left and right of the center of the crack. The y -axis is oriented vertically (along the length of the plate) and is centered so that its positive part reaches the upper boundary, and the negative part reaches the lower boundary of the plate, i.e., $y \in (-L, L)$.

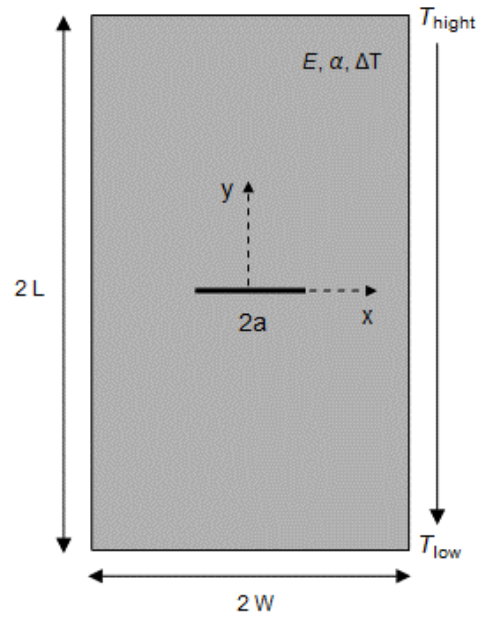


Figure 1. Geometric model of a concrete nanocomposite with a central crack under temperature monotonic loading ΔT

The choice of such a symmetric coordinate system facilitates analytical and numerical analysis and allows the application of simpler models and a clear understanding of the effects of the crack on the temperature distribution and the associated thermal stresses.

BASIC EQUATIONS AND ASSUMPTIONS

Thermal stress

Under monotonically increasing temperature, thermal stress is induced in the material and is determined by the following formula:

$$\sigma_T = E \cdot \alpha \cdot \Delta T \quad (1)$$

where E is the modulus of elasticity, α is the coefficient of linear thermal expansion, and ΔT is the total temperature difference from the upper to the lower boundary of the concrete nanocomposite.

Equation (1) is based on the general principles of thermal expansion theory [13-16] and provides an “average” or global value for the thermal stress that would develop if the entire concrete nanocomposite

were subjected to a constant change in temperature ΔT .

The local thermal stress is determined using the temperature gradient (usually in the y direction, if the temperature field varies mainly in that direction) and is calculated by the formula:

$$\sigma_T(x, y) = E \cdot \alpha \cdot \frac{\partial T(x, y)}{\partial y} \quad (2)$$

This stress depends on the position of (x, y) in the model and reflects the local rate of temperature change.

Stress intensity factor (SIF)

When analyzing SIF in a rectangular plate with finite dimensions (length $2L$ and width $2W$) and with the presence of a central crack of length $2a$, the general formula for calculating SIF is:

$$K_I = \sigma_T \cdot \sqrt{\pi a} \cdot f(a, W) \quad (3)$$

where σ_T are the thermal stresses, a is the crack radius (or half the crack length in the case of a central crack), W is half the plate width, and $f(a, W)$ is a dimensionless correction function depending on the plate dimensions and the crack length.

For small crack lengths relative to the plate width ($\frac{a}{W} \ll 1$), the correction function $f(a, W)$ can be approximated by a Taylor series expansion of the function [18]:

$$f(a, W) \approx 1 + \frac{1}{2} \left(\frac{\pi a}{W} \right)^2 \quad (4)$$

For values of the ratio $\frac{a}{W} \leq 0.01$, we get for the correction function that $f(a, W) \approx 1$, which on the one hand means that the geometric effect is negligible, but on the other hand will help to simplify the calculations. If $\frac{a}{W} \rightarrow \frac{1}{2}$ (the crack is almost half the width of the plate), then $f(a, W) \rightarrow \infty$, equation (5). When the ratio $\frac{a}{W}$ increases and becomes larger than 0.01, expression (4) becomes less accurate and a more precise correction function must be used [20], and the formula should be used:

$$f(a, W) = 1 / \cos \left(\frac{\pi a}{W} \right) \quad (5)$$

Equations (2) and (3) are based on the classical linear elastic fracture mechanics (LEFM) theory developed in [17, 18]. When varying different crack lengths a , the value of K_I will vary linearly with $\sqrt{\pi a}$, which means that longer cracks will also lead to higher stress values. The addition of different nanoparticles to the concrete will change the values of E and α , which will also have an impact on the thermal stresses and ultimately on the value of K_I .

Basic assumptions

- *Homogeneity and isotropy*: The material is assumed to be homogeneous and isotropic.
- *Linear elasticity*: The material behavior remains within the linear elastic region.
- *One-dimensional temperature change*: The temperature change (temperature difference) ΔT is assumed to vary in one direction only (monotonically).
- *Geometric simplicity*: Cracks are modelled with simplified geometric parameters (length).
- *Effect of nanoparticles*: The inclusion of 2% of nano-SiO₂ in the concrete modifies the basic material parameters E and α .

ANALYTICAL AND NUMERICAL SOLUTIONS

Analytical modeling based on linear elastic fracture mechanics (LEFM) was performed and included the generation of special macros in the Wolfram Mathematica software for automation of calculations of thermal stresses and SIF in a concrete composite with or without added 2% of nano-SiO₂. The influence of temperature ΔT and crack length on SIF values was analyzed. A comparative analysis of the obtained results for SIF in a concrete composite with and without added 2% of nano-SiO₂ was also performed. Numerical simulations of thermal stresses and temperature distribution in uncracked and cracked concrete composite with or without added nanoparticles in it are also presented.

Mechanical and thermal characteristics of the concrete composite

The data in Table 1 for the mechanical and thermal characteristics of the concrete composites used for the calculations and simulations are taken from experimental studies published in works [5, 6, 9].

Table 1. Mechanical and thermal characteristics of concrete composites

Type of concrete composite		Elastic modulus, E [GPa]	Coefficient of thermal expansion, α [1/K]
Without nanoparticles		28.149	10×10^{-6}
With nano-SiO ₂		30.655	9.8×10^{-6}

Assumed values of the temperature ΔT and geometry of the concrete composite structural element

The geometry of the rectangular plate (of concrete composites) with a central crack at varying values of the temperature ΔT is presented in Table 2.

Table 2. Assumed values of the temperature ΔT and geometry

Thermal load, ΔT [K]	20 ÷ 200
Plate length, 2L [m]	1
Plate width, 2W [m]	0.5
Initial crack length, 2a [m]	0.001 ÷ 0.1

Temperature distribution in a plate with and without a central crack

- *Calculation of local and total thermal stress:* Macros for numerical modelling using the finite difference method (FDM) and finite element method (FEM) of the temperature distribution in a concrete nanocomposite with and without a central crack, and macros for calculating the total thermal stress (equation (1)) and 2D visualization of the local thermal stress (equation (2)), were generated in the Wolfram Mathematica program. The macros include:

- *Defining the parameters and region of the crack:* First, the values of the main material parameters are defined and set, followed by those for the geometry of the plate and the crack, as shown in Table 2.

- *Boundary conditions:* The boundary conditions are set with fixed temperatures at the upper and lower boundaries T_{high} and T_{low} using Dirichlet conditions: $T[x, -L] = T_{low} = 300$ [K] and $T[x, L] = T_{high} = 400$ [K] and with isolated lateral boundaries (natural Neumann conditions), i.e., $\frac{\partial T(x,y)}{\partial y} = 0$ at $x = \pm W$. The boundary conditions for an isolated crack (with no heat exchange between its walls) are also set using the Dirichlet conditions, i.e., $\frac{\partial T(x,y)}{\partial y} = 0$ at $x = \pm a$. This means that the heat flux through the crack boundaries is zero (insulated walls).

- *Finite element method:* For numerical modelling, the command "NDSolveValue" is used with the option "Method" and type "FiniteElement", i.e., the finite element method is applied to solve the Laplace equation. The command "ContourPlot" is used to numerically model the temperature distribution for the two cases - concrete nanocomposite without and with the presence of a

central crack with length $2a = 0.2$ [m], see Figure 2. It demonstrates that in an uncracked concrete composite, the temperature is distributed evenly, which means that there is a lower concentration of thermal stresses. When the composite material is cracked, heat transfer is disrupted and high temperature gradients appear around the edges of the crack, which leads to an increase in local thermal stresses.

- *Calculation and visualization of thermal stresses:* The total thermal stress is calculated by formula (1), and the local thermal stress is determined using the temperature gradient expressed by formula (2) for different $\Delta T = (20 \div 200)$ [K], Figure 3. The difference in the values of thermal stresses in a cracked concrete composite with and without added 2% of nano-SiO₂ is minimal at low temperature differences as $\Delta T < 70$ [K], while at higher ones this difference increases significantly, as shown in Figure 3. The 2D graphs were generated for the local thermal stresses at $\Delta T = 100$ [K] for both cases – concrete nanocomposite without and with the presence of a central crack with length $2a = 0.2$ [m], Figure 4. It clearly shows that the addition of nano-SiO₂ to the concrete nanocomposite improves its mechanical and thermal properties, but also leads to an increase in thermal stresses in the material. This means that with temperature change, heat spreads faster, which increases the temperature gradient in the material and leads to higher local values of thermal stresses.

Calculation of SIF at different lengths of the central crack at a fixed value of the temperature difference

Special program codes were generated in the Wolfram Mathematica program to automate SIF calculations and to quickly assess the influence of the addition of nano-SiO₂ in the concrete composite (by changing the values of E and α) and the crack length on the values of the stress intensity factor at $\Delta T = 50$ [K]. The results are presented in Table 3. It shows that in the presence of temperature change, concrete composites with 2% of nano-SiO₂ added exhibit higher SIF values compared to ordinary concrete. This phenomenon is observed both at higher and lower temperature differences ΔT , but the effect may manifest itself differently depending on the intensity of the temperature gradient.

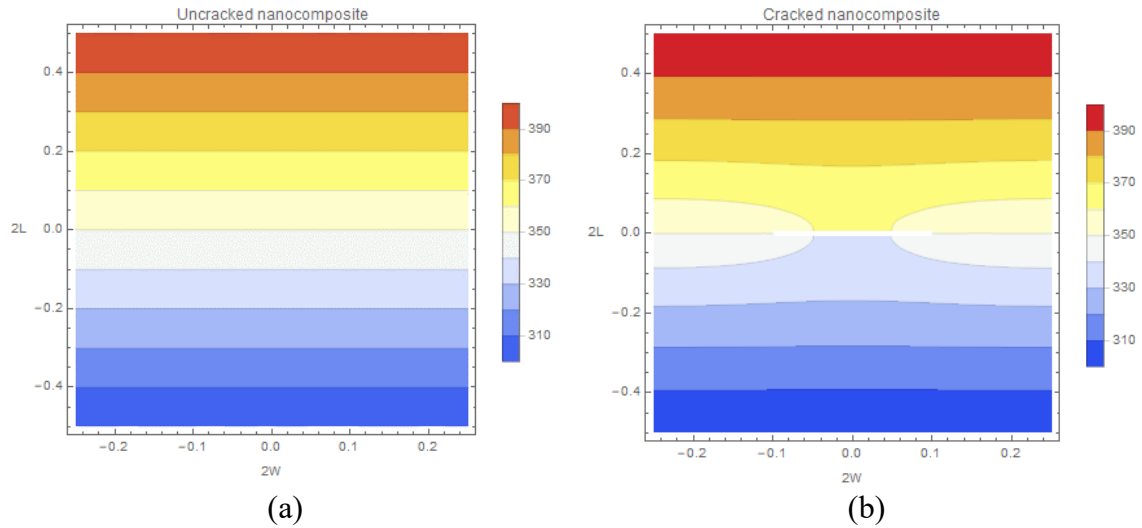


Figure 2. Temperature distribution in (a) Uncracked and (b) Cracked concrete nanocomposite at a fixed value of $\Delta T = 100$ [K].

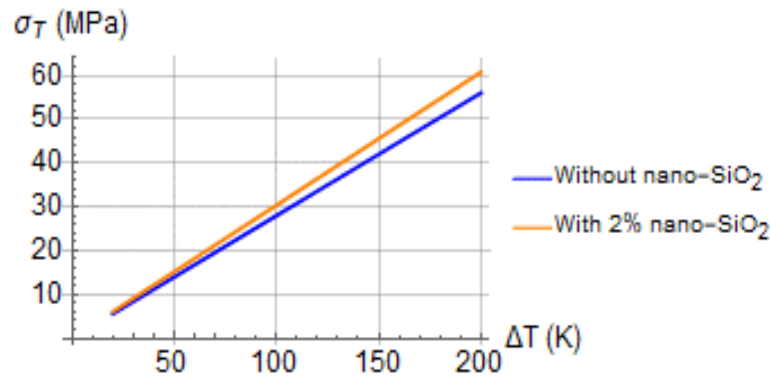


Figure 3. Dependence of the thermal stress on the temperature difference ΔT for cracked concrete composite with / without added 2% of nano-SiO₂.

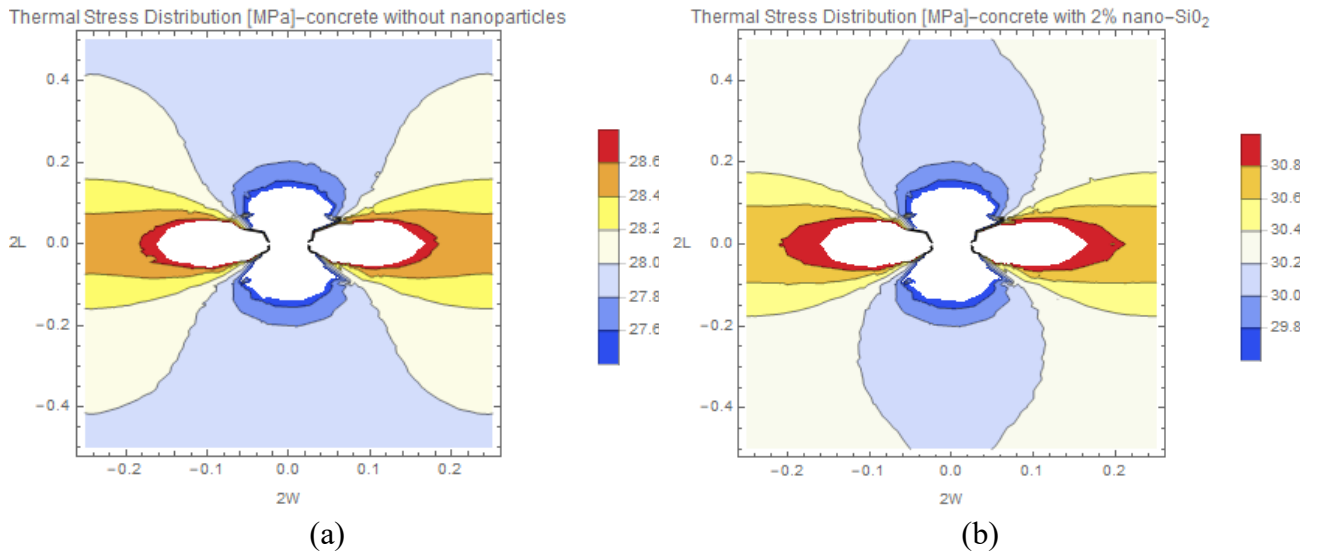


Figure 4. Numerical modeling of local thermal stresses in cracked concrete composite with / without added 2% of nano-SiO₂ at $\Delta T = 100$ [K]

Table 3. SIF calculations

a [m]	K_I [MPa·m ^{1/2}]	
	Concrete without nanoparticles	Concrete with 2% of nano-SiO ₂
0.0005	0.555	0.602
0.001	0.785	0.851
0.0015	0.961	1.043
0.002	1.110	1.204
0.0025	1.241	1.347
0.003	1.360	1.476
0.0035	1.469	1.594
0.004	1.571	1.705
0.0045	1.667	1.809
0.005	1.758	1.908
0.01	2.501	2.714
0.05	6.859	7.441
0.10	25.393	27.552

As ΔT increases, the temperature gradient in the material becomes steeper, which leads to larger local thermal stresses around the crack tip.

INFERENCES FROM THE OBTAINED ANALYTICAL AND NUMERICAL RESULTS

The following conclusions were drawn:

- In uncracked concrete composite, the temperature is distributed evenly, and the concentration of thermal stresses is small. In a composite with a central crack, heat transfer disturbances occur, and high temperature gradients appear around the edges of the crack, which leads to an increase in local thermal stresses.

- Numerical analyses using the FEM confirm the analytical calculations by providing a better understanding of the distribution of thermal stresses in the area around the crack.

- The addition of nano-SiO₂ significantly improves the strength and durability of concrete, but also increases thermal stresses, especially under conditions of rapid temperature change. This means that when designing structures with nano-modified concrete, the increased sensitivity to thermally induced cracking must be considered, and appropriate measures for thermal compensation and temperature gradient control must be implemented.

- The high modulus of elasticity of nano-SiO₂ concrete means that it exhibits greater resistance to deformation, which further increases SIF values. As a result, K_I at high ΔT is larger for nanocomposite concrete compared to ordinary concrete, meaning that cracks are more likely to expand under high temperature loads.

- Adding nano-SiO₂ increases the strength of the concrete, allowing it to withstand higher stresses before cracking. A higher K_I value does not mean that the material is more easily damaged, but that it can accumulate more stress before reaching its critical failure value.

- Concrete with 2% of nano-SiO₂ accumulates higher thermal stresses, which increases the SIF value. However, it has significantly higher compressive strength and elastic modulus, which means that it can withstand higher loads before failure. It is stronger, more resistant to thermal expansion and mechanical stress, making it a better choice for long-lasting and thermally resistant structures.

CONCLUSION

In this study, an analytical and numerical approach is presented to determine the thermal stresses and stress intensity factors (SIFs) in a concrete nanocomposite with a central crack subjected to monotonically increasing temperature. By combining thermal and mechanical models, the influence of both crack length and addition of 2% nano-SiO₂ on the temperature distribution, thermal stress development, and fracture behavior of concrete composites is evaluated. The results show that in uncracked concrete, the temperature distribution remains relatively uniform, resulting in lower thermal stress concentration. In contrast, the presence of a crack leads to localized temperature gradients and higher thermal stresses near the crack tip. Numerical modelling confirms that concrete composite with 2% of nano-SiO₂ accumulates higher thermal stresses due to its higher stiffness—reaching up to 12.8 MPa compared to 10.9 MPa in standard concrete at $\Delta T = 100$ °C. Similarly, SIF values are slightly higher in the nano-SiO₂ composite: for a crack length of 0.01 m, the SIF increases from 25.39 MPa·m^{1/2} (without nanoparticles) to 27.55 MPa·m^{1/2} (with nanoparticles). Although higher SIF values indicate increased stress intensity at the crack tip, the improved strength and elasticity of the nanocomposite ensure that it can sustain greater thermal and mechanical loads before failure.

The developed Mathematica-based macros allow for efficient simulation and analysis, contributing to the practical design of advanced, thermally resilient construction materials. Concrete nanocomposites with nano-SiO₂ are thus a promising solution for durable and energy-efficient structural applications.

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