# ANALYSIS AND CALCULATION OF RESIDUAL STRESS IN CARBON NANOTUBE REINFORCED MAGNESIUM MATRIX COMPOSITES

# ANALÝZA A VÝPOČET REZIDUÁLNÍHO TLAKU V MAGNEZIOVÝCH KOMPOZITECH VYZTUŽENÝCH UHLÍKOVÝMI NANOTRUBICEMI

*Sinian LI* [1], *Yang WANG* [1], *M. H. RÜMMELI* [2], *Jaroslav VLČEK* [3], *Jaromír PIŠTORA* [4], *Michal LESŇÁK* [5]

[1] *Department of Material Processing, Hubei University of Technology, Nahu, Wuhan, 430068, China*

[2] *IFW Dresden, P. O. Box 270116, D-01171, Germany*

[3] *doc., RNDr., CSc., Department of Mathematics and Descriptive Geometry, VŠB-Technical University of Ostrava, 17. listopadu 15, 708 33 Ostrava-Poruba, Czech Republic, tel. (+420) 59 732 4176*
*e-mail: jaroslav.vlcek@vsb.cz*

[4] *Prof., Ing., CSc., Institute of Physics, Faculty of Mining and Geology, VŠB-Technical University of Ostrava, 17. listopadu 15, 708 33 Ostrava-Poruba, Czech Republic, tel. (+420) 59 732 3129*
*e-mail: jaromir.pistora@vsb.cz*

[5] *doc., Dr., Ing., Institute of Physics, Faculty of Mining and Geology, VŠB-Technical University of Ostrava, 17. listopadu 15, 708 33 Ostrava-Poruba, Czech Republic, tel. (+420) 59 732 5206*
*e-mail: michal.lesnak@vsb.cz*

**Abstract**

In this paper we present analysis of interfaces bonding conditions and fracture mechanism in carbon nanotubes (CNTs) reinforced by Mg matrix composites. The CNTs play a very important role in stress transfer, because they can bear larger stress in the process of deformation. We keep the hypothesis that the strengthening of Mg matrix composites is mainly caused by different thermal expansion coefficients in CNTs and matrix. For this reason, the model of enhancement of thermal residual stress was proposed; where its magnitude has been estimated by strengthening model formulas. The results were compared with the experimental author's data from a previous work with good agreement.

**Abstrakt**

V příspěvku jsou zkoumány vazební podmínky a mechanismus narušení na rozhraních magnesiového kompozitu vyztuženého karbonovými nanotrubicemi, které mají významnou roli při transferu napětí v rámci procesu deformace. Vycházíme z hypotézy, že zpevnění Mg matrice je obvykle způsobeno různými koeficienty tepelné roztažnosti vláken a matrice. V tomto smyslu byl navržen model zvýšení reziduálního tlaku. Výsledky byly s dobrou shodou porovnány s dříve získanými experimentálními daty.

**Key words:** CNTs, Mg matrix composites, Thermal residual stress, Strengthening.

## 1 INTRODUCTION

The strengthening mechanism and strengthen prediction of composites are always research hotspots in the field of material science [1]. Jin has studied rules of the elasto-plastic deformation of fibres/particles reinforced composites, and obtained a mathematical model with quite satisfied results [2]. In addition, there was acquired a possibility to predict elasticity of composites using numerical calculations such as the finite element random energy method. However, some basic problems have not been made clear, among others the interface structures of nano-composites, the mechanism of nano-reinforced metal matrix composites (especially by the elasto-plastic deformation), the damage evolution process with energy dissipation or the relation between micro-damage principles and macroscopic properties of nano-reinforced metal matrix composites. Actually, solving these problems is of a great importance for designing a preparation process of composites.

## 2 ESTABLISHMENT OF MODEL

The sub-critical damage of metal matrix composites is related to the fibre breakage under the external force. At present, many experts [3, 4] suppose that improving the mechanical properties of composites depends on the mechanical bonding between the matrix and fibres. If an intensive interaction existed between fibres and their ambient, the reinforcement by fibres would be significantly increased. Therefore, the requirements for the reinforced fibre are as follows:

1. High strength and good toughness of fibre.
2. Tight bonding between fibre and metal matrix.

Mechanical properties of CNTs are very positive: the strength of straight tubes reaches 800 GPa (over 20 times higher than this one for carbon fibre), large aspect ratio (from 5 to 1000 [5]). Thus, we can assume the CNTs as a kind of short fibre with high strength.

Experimental results presented in [6] reveal very good coupling between CNTs and matrix. Since no brittle carbides or other brittle phases are formed, any interface separation or fracture does not occur. The CNTs have a good adhesion to a magnesium matrix. Therefore, assuming CNTs as a type of reinforced fibres that can transfer loading effectively, the acting provided by CNTs can be significant, when the coating of CNTs surfaces improves the coupling between all components.

The interfacial microstructures of composites are different in various systems depending on the method of preparation. They are not fully understood until now, nevertheless, there are seldom studies on the problems of the short fibre reinforced metal matrix composites, where certain simplifications have been made to realize the study of microstructures more convenient. We assumed that the strengthening effect of the CNTs reinforced composites is mainly controlled by the following phenomena [7-9]:

(1) restriction of enhancement to the matrix deformation or to strengthening effect caused by hindrance of dislocation movement in matrix,

(2) load transfer from matrix to strengthening components,

(3) thermal residual stress by deformation enhancement in the matrix produces thermal expansion coefficient mismatch between CNTs and matrix.

According to the compound law, the strength increase of composites can be written as

$$\Delta\sigma = \Delta\sigma_i + \Delta\sigma_r + \Delta\sigma_s \ , \qquad (1)$$

where $\Delta\sigma_i, \Delta\sigma_r, \Delta\sigma_s$ denote residual stress strengthening, fine grain strengthening and dislocation strengthening, respectively.

The residual stress strengthening comes from the different thermal expansion coefficients. When an infinite uniform matrix is supposed, hydrostatic pressure $p$ will act on the reinforcement caused by a thermal expansion coefficient mismatch [10]:

$$p = \frac{2\,\Delta\alpha\,\Delta T\,E_m}{(1+\mu_m) + 2\beta(1-\mu_p)} \quad . \qquad (2)$$

Here $\alpha$, $\mu$, $E$ denote thermal expansion coefficient, Poisson’s ratio and elastic modulus, respectively, $\Delta\alpha = \alpha_p - \alpha_m$, $b = E_m / E_p$. The subscripts $m$, $p$ represents matrix and reinforcement, respectively. Further, for the room temperature $T_R$ the relation $\Delta T = T_p - T_R$ expresses the maximum temperature difference, when the reinforcement growths from cold state to the temperature $T_p$. The plastic deformation can be neglected.

## 2 ANALYSIS OF RESIDUAL STRESS

Consider a small hexahedron element in the coordinate system as in Fig. 1 consisting of two cylindrical surfaces with the distance $dr$, two vertical planes whose angle is $d\theta$ and two horizontal planes with a distance of $dz$. The forces acting on the hexahedron can be projected into the plane $z$ = 0 (Fig. 2), where we formulate the basic problem for the stress function $\varphi(r,z)$ [6], [14]. After some rearrangements, equations for stress components can be expressed as follows (trace amounts and body forces are neglected):

$$\sigma_r = \frac{\partial}{\partial z}\left(\mu\nabla^2\varphi - \frac{\partial^2\varphi}{\partial r^2}\right), \qquad \sigma_\theta = \frac{\partial}{\partial z}\left(\mu\nabla^2\varphi - \frac{1}{r}\frac{\partial\varphi}{\partial r}\right), \qquad \sigma_z = \frac{\partial}{\partial z}\left[(2-\mu)\nabla^2\varphi - \frac{\partial^2\varphi}{\partial z^2}\right],$$

$$\tau_{zr} = \tau_{rz} = \frac{\partial}{\partial r}\left[(1-\mu)\nabla^2\varphi - \frac{\partial^2\varphi}{\partial z^2}\right], \quad \nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{\partial^2}{\partial z^2}, \tag{3}$$

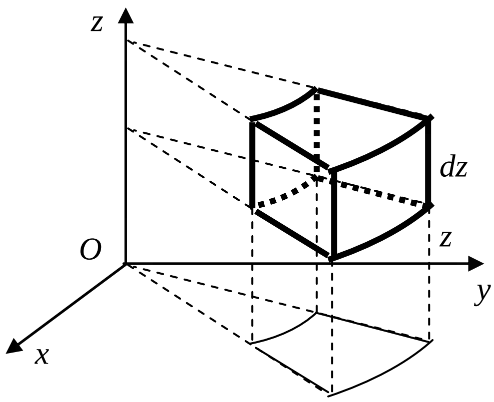


**Fig. 1** Diagram of the volume element

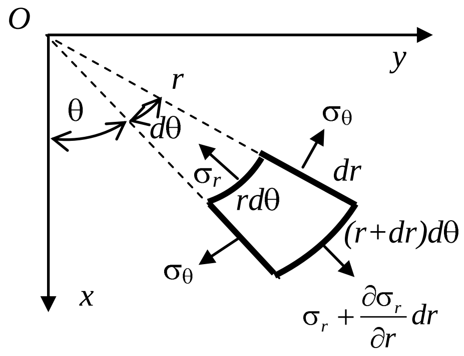


**Fig. 2** Diagram of the loading

where are $\sigma_r$ normal stress in radial directions, $\sigma_z$ normal stress in axial direction; $\sigma_\theta$ normal stress in circumferential directions, $\tau_{rz}$ shear stress acting on cylindrical surfaces along the direction of $z$ axis; $\tau_{zr}$ shear stress acting on horizontal planes in the radial direction.

In particular, assume a solid or hollow cylinder (CNTs) with an arbitrary radius and length. If we denote $q_1$, $q_2$, uniformly distributed pressures acting on the cylindrical surfaces and on the two vertical planar walls, then the stress function $\varphi(r,z)$ can be written as $\varphi = A_1 r^2 z + A_2 z^3$ [11]. Corresponding solutions can be obtained in accordance with the stress boundary conditions:

$$\sigma_r = \sigma_\theta = -q_1, \quad \sigma_z = -q_2, \quad \tau_{zr} = \tau_{rz} = 0 \,. \tag{4}$$

Because the stress $p$ caused by the matrix is related to $q_1$ as $p = -q_1$, one holds

$$\sigma_r = \sigma_\theta = p \,. \tag{5}$$

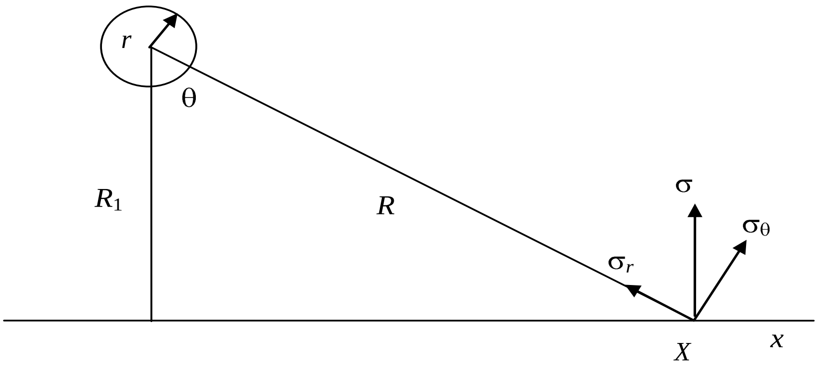


**Fig. 3** Diagram of the loaded interface

Consider the CNTs reinforcement with a radius $r$ and a length $l$ in the matrix neglecting the effect of other deformation sources for simplicity. The hydrostatic pressure $p$ will act on the reinforcement, when this one changes its temperature. Denote $R_1$ the distance between axis of CNTs reinforcement and boundary and θ the angle between radius-vector of arbitrary point $X$ and radius vector of the proximal boundary point (see Fig. 3). Therefore, the normal stress at the point $X$ along the normal direction of grain boundary may be expressed [8] as

$$\sigma = p\cos\theta + p\sin\theta = \sqrt{2}p\sin\left(45^\circ + \theta\right) \tag{6}$$

or

$$\frac{\sigma}{\sqrt{2}p} = \sin\left(45^o + \theta\right) \ . \tag{7}$$

The calculation of the right-hand side of above equation for the angle θ from $0^0$ to $90^0$ shows that $\sigma/p$ increases with the increase of the angle θ in the range of $0^0$ - $45^0$, and, it reaches its maximum $\sqrt{2}$ as the angle θ is $45^0$ and decreases in the rest region. Also, it means that σ and $p$ always have the same sign.

## 3 ESTIMATION OF THERMAL RESIDUAL STRESS

The used material parameters of magnesium matrix and CNTs are referred in [12] Table 1. If the value $T_p$ is given as a sintering temperature of 540 °C, and, $T_R$ is a room temperature of 25 °C, then $\Delta T = T_p - T_R$ = 515 °C. For the data in the first row of Tab. 1 we obtain

$$\Delta\alpha = \alpha_p - \alpha_m = -25.0\times10^{-6} < 0,$$

so that $p < 0$. Because σ and $p$ always have the same sign, we obtain $\sigma < 0$. Thus, the compressive stress caused by the CNTs reinforced phase occurs along the normal direction of grain boundary.

**Tab. 1** Parameters of magnesium matrix and CNTs

| Parameter | Mg matrix | CNTs |
|---|---|---|
| α [ / °C ] | $2.5\times10^{-5}$ | ≈ 0 |
| μ [ - ] | 0.33 | 0.15 - 0.28 |
| $E$ [ GPa ] | 45 | $1.0\times10^3$ |
| ρ [ g/cm³ ] | 1.738 | 1.35 |

Taking $\mu_m = 0.33$, $\mu_p = 0.21$ and $\beta = E_m / E_p$ = 0.045, the relation (2) gives a value of pressure

$$p = \frac{2\Delta\alpha\,\Delta T\,E_m}{1+\mu_m + 2\beta(1-\mu_p)} = -827 \text{ MPa}. \tag{8}$$

The normal stress σ reaches at the angle θ = $45^0$ its maximum $\sigma_{max} = \sqrt{2}p$ = - 1169 MPa.

If no other factors are taken into account, as the higher content of CNTs, greater number of reinforcements or larger enhancement of reinforcements, then the average value of σ,

$$\bar{\sigma} = \sqrt{2}p\left(\frac{\sqrt{2}/2+1}{2}\right) = -998 \text{ MPa}, \tag{9}$$

leads to a volume fraction of reinforcements $V_p$

$$\Delta\sigma = \bar{\sigma}V_p \ . \tag{10}$$

The comparison of the starting and calculated values of the tensile strength is showed in Table 2. The samples contain 0.5 - 1.5 Vol. % of CNTs without perfect enhancement, because they don't have the treatment to electroless plating.

**Tab. 2** Comparison of the experimental and calculated tensile strength

| Data source | Tensile strength [ MPa ] | Volume fraction of CNTs [ Vol. % ] | | | Related to pure Mg matrix |
|---|---|---|---|---|---|
| | | 0.5 | 1.0 | 1.5 | |
| Experiment [6] | σ | 99.78 | 114.23 | 131.21 | 22 - 62 % |
| Numerical model | Δσ | 4.99 | 9.98 | 14.97 | 25 – 75 % |

The tensile strength of pure Mg is about 20 MPa [12, 13]. In the experimental results published in [6] we showed that the tensile strength of Mg composites (without electroless plating) is 23 – 62 % of this value. The theoretical analysis based on the tensile strength caused by the thermal residual stress gives the interval 25 – 75 %. Both these results are very close; nevertheless, the real enhancement is more significant, therefore, the increase of the tensile strength will be higher than the presented values.

## 4 CONCLUSIONS

The strengthening enhancement by CNTs suppresses the dislocations caused by the thermal residual stress, because CNTs hinder the main crack extension. In the presented theoretical calculation, only the effect of thermal residual stress was considered in a simplified theoretical model, moreover, no interaction between CNTs was assumed. On the other hand, the dispersible uniformity of CNTs has not been solved perfectly in experiments, and, the addition amounts of CNTs were very small. Notwithstanding, the strengthening enhancement calculated by the thermal residual stress model exhibits a good agreement with experimental results, so that the thermal residual stress model can sufficiently explain the strengthening mechanism of CNTs reinforced Mg matrix composites.

**REFERENCES**


[1] KLEIN, T. W. (transl.), YU, Yongning et al. *Introduction to Metal Matrix Composites*, 1st ed., Beijing, Metallurgical Industry Press, 1996.

[2] JIN Ling. Finite Element Analysis of Micro-Stress. *Metal Matrix Composites*. *Journal of Shanghai Institute of Technology*. 2002, 2, No. 1, pp. 12-16. (*in Chinese*)

[3] TREASY, M. M. J., EBBSEN, T. W., GIBSON, J. M. Exceptionally high Young's modulus observed for individual carbon nanotubes. *Nature*, 1996, pp. 381-678.

[4] CAI, L., Microstructure and heterogeneous nucleation phenomena in cast SiC particle reinforced magnesium composite. *Material Science and Engineering*, 2000, 828A, p. 232.

[5] IMAMURA, H., SAKASAI, N. Hydriding characteristics of Mg-based composites prepared using a ball mill. *Journal of Alloys and Compounds*, 1995 (231), pp. 810-814.

[6] LI, Sinian, SONG, Shouzhi, YU, Tianqing et al. Properties and Microstructure of Carbon Nanotubes/Magnesiuum Matrix Composites, *Journal of Wuhan University of Technology*, 2003, Vol. 25 (11), pp. 1-4. (*in Chinese*)

[7] LEI, Xiujuan. *Mechanical Properties of Nanocomposites*. Xi An, Northwest Industrial University Press, 2001.

[8] LEI, Xiujuan. *Mechanical Properties of Nanocomposites*. Wu Han, Hubei University of Technology Press, 2004.

[9] CHUA, B. W., LU, L., LAI, M. O. Influence of SiC Particles on Mechanical Properties of Magnesium Based Composite. *Composite Structures*, 1999, 47, p. 595.

[10] KANG, Guo-zheng., GAO, Q. Stress distribution and deformation characteristics of matrix in short fiber reinforced metal matrix composites. *Acta Materiae Compositae Sinica*, 2002, 02 (5).

[11] PIGNEY, A., LAURENT, C. H., ROUSSET, A. Synthesis and Characterization of alumina matrix nanocomposites containing carbon nanotubes, *Engineering Materials*, 1997, 132, pp. 743-746.

[12] LIM, Suk-won, TSUNEMICHI, Imai, YOSHINIRI, Nishida, et al. High Strain Rate Super Plasticity of TiC Particulate Reinforced Magnesium Alloy Composite by Vortex Method. *Scripta Metallurgica et Materialia*, 1995, 32 (11), pp. 1713-1717.

[13] BRASCZYNSKA, K. N., LITYNSKA, L., ZYSKA, A, et al. TEM analysis of the interfaces between the composites in magnesium matrix composites reinforces with SiC particles, *Material Chemistry and physics*, 2003, 81, pp. 326-329.

[14] TIMOSHENKO, S. P., GOODIER, J. N. *Theory of Elasticity*. New York, MacGraw-Hill, 1970.

### RESUMÉ

Zpevnění hořčíkového kompozitu malým objemovým podílem uhlíkových nanotrubic (0,5 – 1,5 %) zabraňuje šíření mikrotrhlin. V příspěvku je studován teoretický model zpevňujících účinků, který vychází z rozdílnosti koeficientů teplotní roztažnosti Mg matrice a karbonových nanotrubic. Je prezentována formule pro střední hodnotu přetvoření, z níž jsou vypočtena procentuální navýšení tahové pevnosti ve srovnání s původní (nezpevněnou) matricí – viz vztahy (2), (9) a (10).

Výsledky jsou s dobrou shodou porovnány s experimentálními daty publikovanými v práci [8], z níž jsou rovněž převzaty číselné hodnoty použité ve výpočtech. Závěry ukázané v Tab. 2 jsou diskutovány se zřetelem k jistým omezením, uplatněným jak v experimentech, tak při koncipování teoretického modelu.

### ACKNOWLEDGEMENTS

This project is supported by the Wuhan Chen Guang Project (Grant No. 20015005030), the Hubei Province Natural Science Funds (Grant No. 2002AB49).