Journal of Materials Science and Engineering B 4 (12) (2014) 353-357
doi: 10.17265/2161-6221/2014.12.003

Evaluation of Dispersion Based Calculations Compared to the Experimental Compressive Strength Results of CNT/6063Al Composites

Bedri Onur Kucukyildirim and Aysegul Akdogan Eker

Department of Mechanical Engineering, Yildiz Technical University, Istanbul 34349, Turkey

Received: December 01, 2014 / Accepted: December 21, 2014 / Published: December 25, 2014.

Abstract: Nowadays, it is vital to predict strength results of composites in advance of manufacturing process to reduce testing costs; especially in carbon nanotube (CNT) reinforced metal matrix composites. Therefore, compressive mechanical properties of fabricated CNT reinforced aluminum (Al) matrix composites are investigated and compared with the calculation results of dispersion based prediction models. First of all, CNT/6063 Al composites are fabricated by vacuum assisted infiltration of molten 6063 Al alloy into the CNT preform. Then, compressive mechanical properties of these composites are determined. Eventually, model calculations and experimental results are visualized by plotting comparison graphs. As a result, correlation between prediction models and experimental results are established and potential results of difference between these results are discussed.

Key words: Carbon nanotube, metal matrix composite, mechanical properties, prediction model, dispersion strengthening.

Nomenclature

b:	Burger's vector
c:	Composite
f:	Fiber
G:	Shear modulus
$\langle L \rangle$:	Average interparticle spacing
m:	Matrix
M_T:	Taylor factor
p:	Moduli
$\langle r \rangle$:	Average particle radius
V:	Volume ratio
Wt:	Weight
y:	Yield

Greek Letters

η:	Fiber coefficient
α:	Randomness of the discontinuous fibers
ξ:	Measure of the reinforcement.
$\Delta\tau_y$:	Increase in shear stress
$\Delta\sigma$:	Strength difference
$\Delta\tau$:	Shear stress difference

1. Introduction

Carbon nanotubes (CNTs) are known as one of the strongest and stiffest materials discovered in terms of tensile strength and elastic modulus. Various simulation studies and experiments prove excellent mechanical properties of CNTs [1-4]. The mechanical behavior of composites is related to the load sharing between matrix and reinforcement [5]. The proportion of the load carried by the reinforcement is independent from the overall carried load; however, strength of the composite depends on factors such as volume fraction of reinforcement, shape, orientation. Prediction of the strength results of composites in advance of manufacturing process to reduce testing costs is important. Importance of prediction comes into prominence when expensive materials such as CNT are used as reinforcement. In addition, further costs are

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Corresponding author: Bedri Onur Kucukyildirim, Ph.D., researcher, research fields: composites, shapememory alloys, carbon nanotubes and biomaterials. E-mail: kucukyil@yildiz.edu.tr.

discussed in the fabrication of metal matrix composites. Therefore, many studies were carried on about the strengthening mechanisms of CNT reinforced aluminum (Al) matrix composites [6]. Some of these studies compared the experimental data with the prediction model results for evaluating only tensile strength and elastic modulus of these composites [7-10]. In addition to these studies, our previous study presented the experimental compressive strength data of vacuum infiltrated CNT/Al composites compared with the various prediction models [11]. Three models, Halpin-Tsai equations, shear lag theory and thermal mismatch theory for yield strength were applied and the most matching model was determined in this previous study. In this recent study, compressive mechanical properties of fabricated CNT preform reinforced 6063 Al matrix composites are compared with the calculation results of a modified Halpin-Tsai model developed with the dispersion based prediction model in order to include the effect of dispersion strengthening feature of CNTs.

2. Material and Method

In this study, fabrication of CNT/Al composites by vacuum assisted infiltration method using CNT preform reinforcement is realized successfully. Firstly, industrial type MWCNTs (10-30 nm diameter; around 2.1 g/cm^3 true density) with a purity rate of over 85% are chemically functionalized with 65wt% HNO$_3$ by reflux. Next, preforms are produced using these CNTs, poly vinyl alcohol (PVA) as a pore forming agent and colloidal silica (10-20 nm grain size; around 1.20 g/cm^3 density) as binding agent. Afterwards, one of the most used metal matrix materials; 6063 aluminum alloy is infiltrated into these preforms by using vacuum assisted casting machine. After fabrication, compressive test specimens are prepared and tests are carried out according to ASTM E9 [12] standard using universal mechanical testing machine. Usually, in a compressive test, the strain increases with the sample deformation without reaching a limit and ultimate compressive strength is specified with a slope starting from a specified offset point like determination of yield point. In the study, yield stress is taken as the elastic limit in accordance with Pérez-Bustamante et al. [13]. Our main mathematical expression for the prediction of composite strength is modified Halpin-Tsai, which is given in Eq. (1) [10]:

$$\frac{p}{p_m} = \frac{1+\xi\eta V_f}{1-\eta V_f};\eta = \frac{\dfrac{\alpha p_f}{p_m}-1}{\dfrac{\alpha p_f}{p_m}+\xi} \tag{1}$$

where, p represents the moduli such as elastic modulus, strength or shear modulus p_m and p_f are the corresponding matrix and fiber moduli, respectively. Model is modified with the orientation factor parameter alpha α to account for the randomness of the discontinuous fibers where ξ is the measure of the reinforcement.

Moreover, as a novelty, we use dispersion hardening model to include dispersion strengthening effect of CNTs [5]. For this reason, the increase is applied by adding yield strength difference given in Eq. (2):

$$\Delta\tau_y = 0.84\frac{1.2Gb}{2\pi\langle L\rangle}\ln\frac{\langle r\rangle}{b};$$

$$\langle r\rangle = \frac{d}{2(3/2)^{1/2}};\langle L\rangle = \left(\frac{\pi\langle r\rangle^2}{V_f}\right)^{1/2} \tag{2}$$

where, $\Delta\tau_y$ is the increase in shear stress, $\langle L\rangle$ the average interparticle spacing and $\langle r\rangle$ the average particle radius. The increase in the shear stress can be found in yield strength difference form by using Eq. (3):

$$\Delta\sigma_y = M_T\Delta\tau_y \tag{3}$$

where, M_T is the Taylor factor.

3. Results and Discussion

3.1 General Remarks

Starting with the matrix material specimens, compressive tests are applied to composite material specimens with the same parameters as mentioned in

ASTM E9 [12]. Yield strength and relative densities of all specimens are given in Table 1 with standard deviations for strength values.

It is possible to see the mechanical enhancement by looking to the experimental results given in Table 1. Modeling parameters are given in Table 2 including the *E* and *T/A* labels tagged as superscript to parameter names indicating that this parameter is experimental or theoretical from another study, respectively. All parameters can be found in our previous model comparison study [11].

In fact, the function of strength consists of various components as shown in Eq. (4). Some of them have positive effects while some of them have negative effects (e.g., agglomeration, voids). However, in our total yield strength, positive ones are considered according to the Eq. (5):

$$f(\sigma_C) = \{\sigma_{C\,Mod.Halpin-Tsai}, \sigma_{C\,Dispersion}, \dots\} \tag{4}$$

$$\sum \sigma_y = \sigma_{C\,Mod.Halpin-Tsai} + \sigma_{y\,Dispersion} \tag{5}$$

In Fig. 1, it is possible to see curves calculated according to mathematical models and our experimental results with standard deviations according to the Eq. (5).

Our experimental results are well-matched with the Halpin-Tsai calculations; however, with the exception of 0.75wt% CNT reinforced composite strength results, they are higher than expected due to some factors such as shape factor and orientation factor. When the dispersion strengthening effect is added, it is found out that calculation results are matching with the 0.25wt% CNT reinforced composite strength results. Apart from this, calculation results are over experimental results.

The main reason for this situation is related to the faults in materials that increase with the increase of CNT ratio. Regarding to the fabrication method, it becomes more difficult to disperse CNTs alone homogeneously in the matrix with the increase of the reinforcement ratio.

Table 1 Compressive yield strength values and relative densities of CNT/6063 Al composites.

Composition of specimens	Average σ_y (MPa)	Relative density (%)
6063 Al matrix	42 ± 2.1	99.59
0.25wt% CNT/6063 Al	127 ± 12.6	99.02
0.50wt% CNT/6063 Al	148 ± 16.6	98.86
0.75wt% CNT/6063 Al	151 ± 13.2	98.41

Table 2 Parameters for modified Halpin-Tsai and dispersion based model calculations.

Parameter [11]	Values
Strength of 6063 Al: σ_{6063Al}^{E} (MPa)	42
Strength of CNT: $\sigma_{CNT}^{T/A}$ (GPa)	100
Poisson ratio: $\gamma_{6063Al}^{T/A}$	0.33
Shape factor of CNTs: $s_{CNT}^{T/A}$	100
Strength of alumina: $\sigma_{Al2O3}^{T/A}$ (MPa)	5,500
Shape factor of alumina: $s_{Al2O3}^{T/A}$	5
Average length of CNTs: λ_{CNT}^{E} (µm)	20
Average diameter of CNTs: d_{CNT}^{E} (nm)	20
Orientation factor of CNTs: $\alpha_{CNT}^{T/A}$	0.166667
Burgers vector: $b^{T/A}$ (nm)	0.286
Shear modulus of Al: $G_{6063\,Al}^{T/A}$ (GPa)	25.8
Taylor factor: M_T [14]	3.1

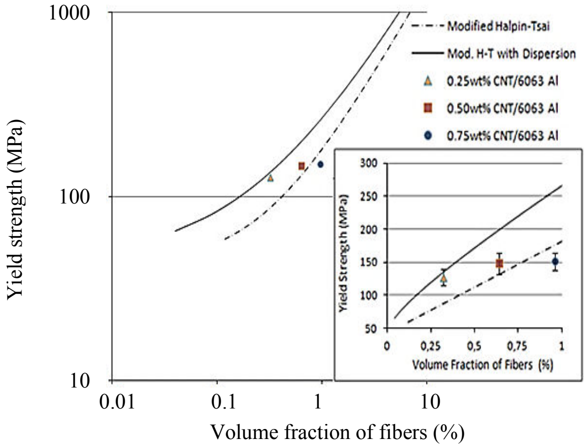

Fig. 1 Experimental and plotted curves of calculated values for yield strength of CNT/Al composites.

The Halpin-Tsai equation is a semi-empirical method by which the yield strength of composites can be calculated for fibers of unit aspect ratio. In modified Halpin-Tsai equation, the geometry factor, which depends on the boundary conditions such as fiber geometry, distribution and loading conditions are incorporated into the model.

The modified Halpin-Tsai model demonstrates the significant effect of reinforcement geometry alone on the strength properties of a unidirectional oriented and orthotropic composite at both constant volume fraction and packing geometry; changing from a sphere to a long fiber gives an order of magnitude or more increase in strength for both a unidirectional and a randomly distributed reinforcement depending on the constituent.

It is observed that experimental results are mostly above the modified Halpin-Tsai prediction curve. This relation is mainly related to different strengthening mechanisms. The presence of CNTs leads to dispersion strengthening of the matrix owing to their nano size. Even though CNTs are small fibers, they are not coherent with the matrix with exception of a far amount of interface; they do not chemically react with the matrix. They block the movement of dislocations and bring out the dispersion strengthening effect of composites as expected.

Difference between experimental and modified Halpin-Tsai calculation results is related to the average CNT dimension and length parameters. With the exception of dispersion strengthening effect, our CNTs are supposed to have higher length/diameter ratio *c* than the accepted parameter for the calculation. Furthermore, the length/diameter ratio will be even higher than estimated value considering the agglomeration of CNTs. However, if we consider the dispersion strengthening effect and search for the reason of the difference between compound function and experimental results, agglomeration of CNTs and often-ignored voids show up as the main and probable cause. It is possible to show the decreasing relative density as an evidence of void formation in this study.

4. Conclusions

In this study, compressive mechanical properties of fabricated CNT preform reinforced 6063 Al matrix composites are compared with the calculation results of a modified Halpin-Tsai model developed with the dispersion based prediction model in order to include the effect of dispersion strengthening feature of CNTs.

The mechanical enhancements of the composites are interrelated with the bridging and pulling-out of CNTs in the fracture surfaces. All of these mechanical aspects are considered in the modified Halpin-Tsai equation.

However, modified Halpin-Tsai equation remains incapable for the strength prediction calculations of CNT reinforced MMCs.

By the compound function of two equations, it is possible to include the dispersion strengthening effect.

Furthermore, it is observed that upper strength limit of the composites can be drawn by the developed model.

Acknowledgments

Experimental part of this research has been supported by Yildiz Technical University Scientific Research Projects Coordination Department; Project number: 28-06-01-01.

Thanks to Dr. Kerem Altug Guler, and Mr. Alptekin Kisasoz from Yildiz Technical University, BCACT: Balkan Center for advanced casting technologies, Istanbul, Turkey for their technical support.

Additional Information

This invited article has been presented in IMSP'2014 International Materials Symposium organized by Pamukkale University between October 15 and 17, 2014 in Denizli.

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