# Strain rate and temperature dependent mechanical properties in CNT-

## reinforced magnesium composites

### †\*Xia Zhou, Xiaoxia Liu, and Mengqi Shen

State Key Laboratory of Structural Analysis for Industrial Equipment, Department of Engineering Mechanics, Faculty of Vehicle Engineering and Mechanics, Dalian University of Technology, Dalian 116024, China.

\*Presenting author: zhouxia@dlut.edu.cn †Corresponding author: zhouxia@dlut.edu.cn

#### Abstract

Magnesium (Mg) matrix nanocomposites containing carbon nanotubes (CNTs) have good application prospects in aerospace, automotive, military and other fields due to their high specific strength, specific stiffness and excellent damping capacity [1]. However, the main research efforts were focused on CNT-reinforced polymer matrix composites, while the relative works on metal matrix composites are relatively rare, especially for magnesium [2] in the past decades. No attempt has been done with the strain rate and temperature effect on the mechanical properties of CNT/Mg composites. This paper aims at investigating the dynamic mechanical response of Ni-coated CNT reinforced Mg composites (CNT-Ni/Mg) at different temperatures by using molecular dynamics (MD) method. The CNT-Ni/Mg composite models with various CNT diameters are constructed and dynamic tensile properties of the composites have been investigated at different strain rates and temperatures. The MD simulation results shown in Figure 1 indicate that Ni-coated CNT can improve the mechanical properties of the composite effectively. Compared with the single-crystal Mg and uncoated CNT/Mg composite, the yield stress increases by 19.84% and 3.11%, the elastic modulus of the composite increase by 25.36% and 3.65% respectively at 300K and a strain rate of  $1 \times 10^{9}$ s<sup>-1</sup> The calculated elastic modulus of the composite is also consistent with the prediction based on the rule-of-mixture. The mechanical properties of CNT-Ni/Mg are still better than those of the monolithic Mg and uncoated CNT/Mg at a higher temperature. In addition, the composite exhibits a strong temperature softening effect and a positive strain rate sensitivity when the strain rate is larger than  $6 \times 10^9$  s<sup>-1</sup>. At the same time, the yield of the composites is prone to occur at small strain levels under the coupling effect of low strain rate and high temperature (Figure 2). The failure of the composites at the nanoscale is mainly attributed to the atomic disorder, micropore and dislocation formation in the Mg matrix and the fracture of CNTs near the micropores (Figure 3).

**Keywords:** CNT-Ni/Mg composite, Molecular dynamics simulation, Temperature, Strain rate, Mechanical properties.

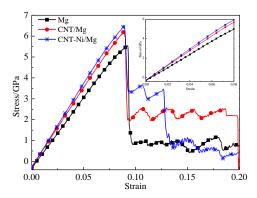
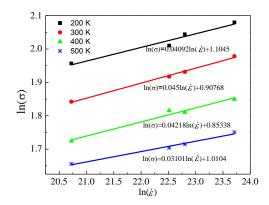
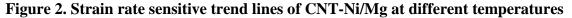


Figure 1. The tensile stress-strain curves of Mg, CNT/Mg and CNT-Ni/Mg at 300 K and  $10 \times^9 \text{ s}^{-1}$ .





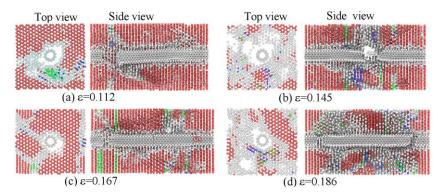


Figure 3. Fracture snapshots of CNT-Ni/Mg at different strains and different temperatures: (a) 500 K,  $1 \times 10^9$  s<sup>-1</sup>; (b) 400 K,  $6 \times 10^9$  s<sup>-1</sup>; (c) 300 K,  $8 \times 10^9$  s<sup>-1</sup>; (d) 200 K,  $2 \times 10^{10}$  s<sup>-1</sup> (red:HCP, green:FCC, blue:BCC, gray: Other)

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### References

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