**Towards in a new equation for the interfacial failure of nanocomposites**

**S. V. Kallivokas1,2,\*, A. P. Sgouros2, D.N. Theodorou2**

1 Centre for Research and Technology Hellas/Hellenic Institute of Transport,

6th Km Charilaou - Thermi Rd. Thermi, Thessaloniki Macedonia 57001 Hellas

2 School of Chemical Engineering, National Technical University of Athens (NTUA), GR-15780 Athens, Greece

*\* skallivokas@certh.gr*

**ABSTRACT**

Interfacial shear strength (IFSS) is a key property in the design of composites and nanocomposites; thus, a method for its “bottom up” estimation from the chemical constitution of matrix and filler would be highly beneficial.

In this work we propose a new way to calculate the IFSS from atomistic simulations through a statistical mechanics and kinetics approach.1 This methodology is applicable in both periodic and aperiodic systems. It is based on conducting shear deformation simulations of the interface over a wide range of temperatures and shear stresses and interpreting the results in the framework of an extended Boltzmann-Arrhenius-Zhurkov kinetic equation.2 Thus, it is able to capture both the long time (rare event) and short time characteristics of interfacial failure. As realistic models to test our new methodology and equation we use epoxy/graphene nanocomposites with three types of graphene: pristine, defective, and oxidized.3,4 In addition to the IFSS, we calculate the local shear modulus, which is comparable to the Winkler modulus, and validate our results against experiment.5

**KEYWORDS:** Adhesion, Fracture, Composite materials, Interfaces, Rare event statistics

**REFERENCES**

1 S. V. Kallivokas, A. P. Sgouros and D. N. Theodorou, *Phys. Rev. E., 2020, 102, 030501(R)*

2 S.N. Zhurkov, *Int. J. Fract. Mech.*, 1965, 1, 311–322.

3 S. V. Kallivokas, A. P. Sgouros and D. N. Theodorou, *Soft Matter*, 2019, **15**, 721–733.

4 A. K. Geim and K. S. Novoselov, *Nat. Mater.*, 2007, **6**, 183–191.

5 C. Androulidakis, E. N. Koukaras, M. G. Pastore Carbone, M. Hadjinicolaou and C. Galiotis, *Nanoscale*, 2017, **9**, 18180–18188.