3rd International Conference on Self-Healing Materials
Bath, UK. 27-29 June 2011

# NUMERICAL SIMULATION OF MICRO-CAPSULE BASED SELF-HEALING MATERIALS

Sze Dai, Pang[1], Phuoc Thao, Tran Diep[1] and Ser Tong, Quek[1]

[1]Department of Civil Engineering, National University of Singapore
Block E1A, #07-03, 1 Engineering Drive 2, Singapore 117576
Email: cvepsd@nus.edu.sg

**Keywords:** Self-healing, Healing Efficiency, Biomimetics, Representative Volume Element

## ABSTRACT

### Introduction

In 2001, White et. al. [1] reported on a novel smart material that is capable of self-sensing and repairing micro-cracks in quasi-brittle materials by micro-encapsulating and embedding healing agent host polymer matrix to create micro-capsule based self-healing material (SHM). Since then, there have been further reports on experimental parametric studies to vary the size and volume fraction of capsules to improve its healing efficiency and up to 80% recovery in fracture toughness have been reported [2]. To complement the experimental efforts to utilize the full potential of the SHM, a predictive tool is necessary to conduct cost-effective parametric studies and also to provide detailed information of the underlying mechanisms. The goal of this present study is to develop a numerical micro-mechanical model using homogenization technique with Representative Volume Element (RVE) concept to characterize the mechanical properties of SHM including its healing efficiency.

### Remarks from experimental data

Brown et al. [2] experimentally determined material properties, such as Young's modulus, $E$, strength, $\sigma_f$, fracture toughness $K_{IC}$ and healing efficiency in terms of recovered fracture toughness, $\eta$, of the SHM using 180μm-diameter micro-capsules at different volume fractions. The test results show monotonic trends of decline in both $E$ and $\sigma_f$ with an increase in volume fraction, $f$. In particular, the effective strength of SHM drops to less than 50% compared to that of the host matrix when $f$ is increased to 22%, making the composite more vulnerable. In contrast, a rise in the micro-capsule concentration leads to a rise in the effective fracture toughness until a peak value is reached at $f$=17%. Analysis of SEM photos suggests that shear yielding in the matrix caused by the embedded micro-capsules is likely the governing mechanism for the toughening of the composites.

### Numerical model

Three-dimensional finite element simulations using both single-particle RVE (SP-RVE) and multiple-particle RVE (MP-RVE) approaches were conducted for 3 volume fractions of 6%, 11% and 17%. At each of the 3 volume fractions of the MP-RVEs, the average value is computed based on 6 realizations to account for the randomly placed micro-capsules. The size of the SP-RVE is varied based on the volume fraction being investigated while the size of the MP-RVE is kept at a constant size of 750μm, which is more than 4 times the size of the micro-capsule. The matrix is modelled as a homogeneous material and its crack-softening behaviour is simulated using the smeared crack model. The fluid-filled micro-capsules are modelled as voids as the micro-capsules are more three orders of magnitude softer than the matrix, to have any significant contribution to the elastic response of the composite; preliminary studies with micro-capsule modelled as an elastic shell enclosing a Neo-Hooken material has yielded almost identical elastic response. The shear-yielding effect of the micro-capsules on the post-elastic behaviour of the composite is modelled by introducing shear retention in the smeared crack model. As the matrix toughening is attributed to the micro-capsules, the shear retention factor has to vary with the volume fraction of the micro-capsules. Two parametric studies with full and no shear retention are also conducted in this study for comparison.

The mechanical properties of the virgin SHM, which include Young's modulus, strength and fracture toughness, are investigated by applying displacement-controlled uniform traction on two opposite

planes of the RVEs. The healed properties of the SHM are subsequently investigated by replacing the damaged elements obtained from the previous step with new elements that represent the cured healing agent.

## Results and discussion

The comparison of the predicted material properties of SHM based on the RVE with the experimental test results is shown in Figure 1. Both $E$ and $\sigma_f$ of SHM can be predicted well using either MP-RVE or SP-RVE approaches with less than 10% error, validating the use of SP-RVE to predict elastic properties of particulate composites for low volume fraction.

For the prediction of fracture toughness, the trend observed from experiments using well-bonded micro-capsules [2] is similar to the trends of RVE simulations with shear retention, among which the model with varying shear retention factors provide the best estimation with less than 10% of deviation. RVE models without shear retention, including SP-RVE and MP-RVEs with zero shear retention factor, are unable to simulate the toughening effect of SHM. The $K_{IC}$ predicted from these models exhibits a trend analogous with that received from the experiments with poorly bonded micro-capsules. The proposed approach of using MP-RVE with varying shear retention factor for the matrix is used for the investigation of the fracture toughness recovery after healing which shows a good match with the experiments (Figure 1).

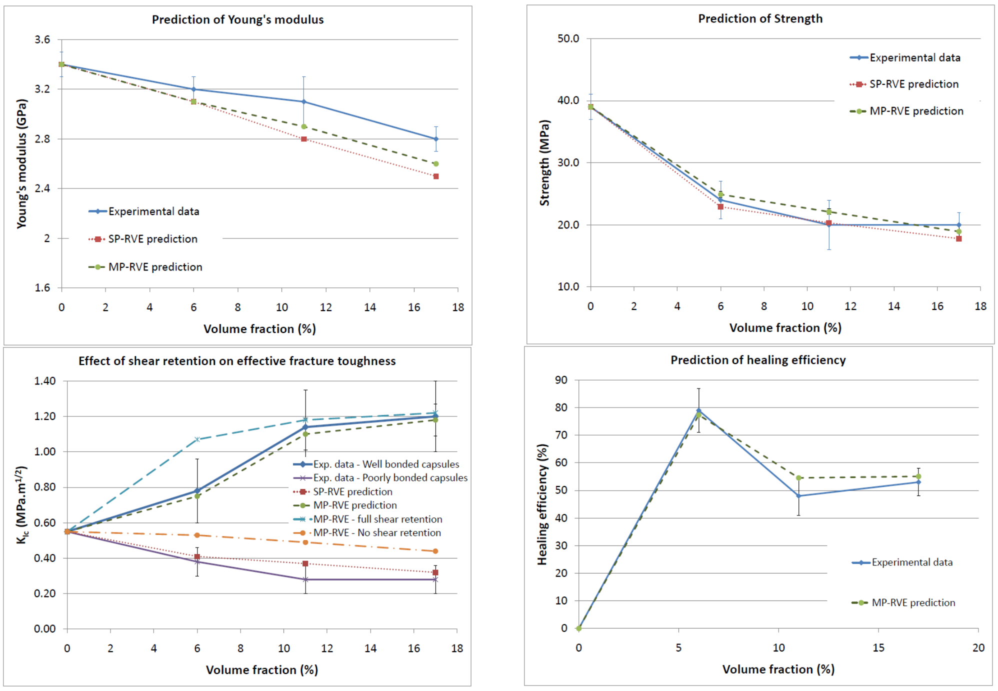

Figure 1: Comparisons of mechanical properties of SHM from experiments and numerical simulations.

## Conclusion

In this study, RVE approaches using voids and shear retention modification in matrix is adopted to simulate mechanical response of SHM and predict its healing efficiency. MP-RVE approach generates good prediction for both the mechanical properties and healing efficiency of SHM while SP-RVE approach is only limited to the prediction of elastic properties.

## REFERENCES

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