

Finite Element Based Modeling of Micro-mechanical Response of Computer Simulated 'Realistic' Microstructures with Spatial Heterogeneity at Different Length Scales

A. Sreeranganathan, H. Singh, A.M. Gokhale

School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, GA-30332

In the recent years, there have been numerous studies on computer simulations of micro-mechanical response of material microstructures. Most of these investigations assume simple shapes for the microstructural feature of interest (particles, voids, etc.) [1, 2] and/or utilize small microstructural segments (typically one field of view or so) [3] as representative volume element (RVE) of microstructure. Such simulations are useful for simple parametric studies, but do not represent micro-mechanical response of complex heterogeneous material microstructures. The assumption that a single microstructural field of view serves as the representative volume element clearly breaks down for microstructures containing clustering over length scales much larger than a single microstructural field. Technologically important materials such as discontinuously reinforced Al- and Ti-alloy composites fall in this category. This is illustrated in Figure 1(a) where a montage image of 125 contiguous microstructural fields of view of an Al/SiC_p composite with long-range spatial heterogeneity is shown. A single field of view from the montage is shown in Figure 1(b), which fails to capture the clustering of particles in the microstructure. It is also known that in these materials, the mechanical properties are affected to a large extent by the spatial distribution of the reinforcement particles in the matrix [4-6]. Therefore, it is of interest to explore new methodologies for reliable simulations of micro-mechanical response of such materials. It is of added interest to quantify the spatial distribution and clustering of the reinforcement phase in a microstructure in terms of a few mathematical parameters. This information can be used to simulate 'realistic' microstructures that are statistically similar to the real microstructures. Figure 2 shows such a simulated microstructure statistically similar to the real microstructure in Figure 1(a). It is also possible to create 'virtual' microstructures with varying degrees of clustering, or in effect, varying process conditions by changing these numerical parameters. The detailed methodology followed for creating simulated and 'virtual' microstructures from these parameters is described in another contribution.

In this contribution, we make use of finite element based modeling to study the micro-mechanical behavior of real and virtual microstructures. The SiC particles are assumed to be perfectly elastic and elastic-plastic behavior is assigned for Al matrix. The interface between the matrix and the reinforcement particles is assumed to be perfect. The microstructural frame is embedded in a homogeneous composite material with the mechanical behavior to be determined iteratively to avoid edge effects. Periodic boundary conditions are used for the analyses. An FEM mesh of a microstructural image is shown in Figure 3. The overall mechanical behavior of the composite is determined by volume averaging the stress/strain values at each integration point. The effect of clustering (or processing conditions) on the mechanical behavior of the material is investigated by studying microstructures with varying degrees of clustering. The simulations are used to predict the mechanical behavior of Al/SiC_p composites with a specific set of processing conditions. Dependence of the representative volume element required for accurate representation of the whole microstructure on the degree of clustering is studied.

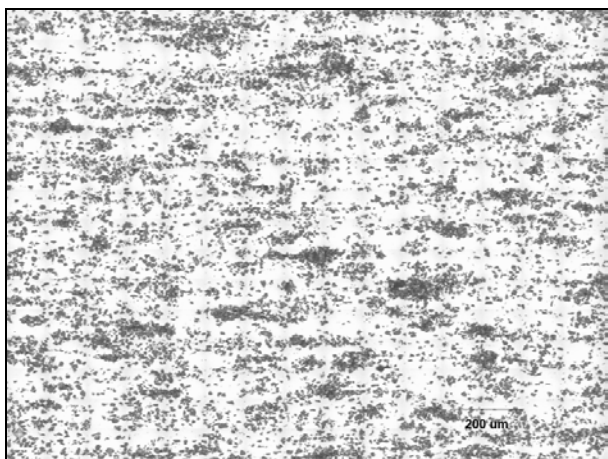


Figure 1a: Montage of 125 fields of view

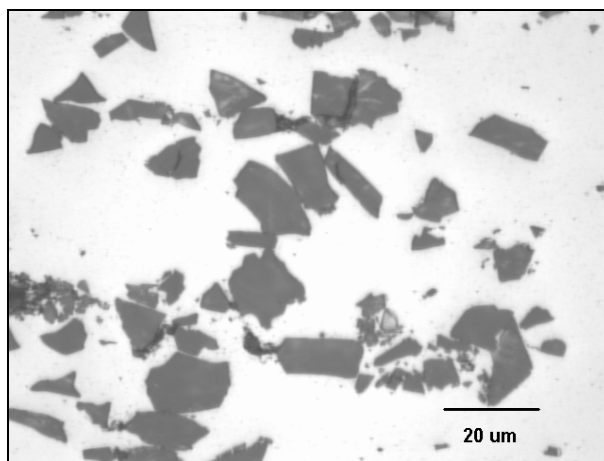


Figure 1b: Single field of view

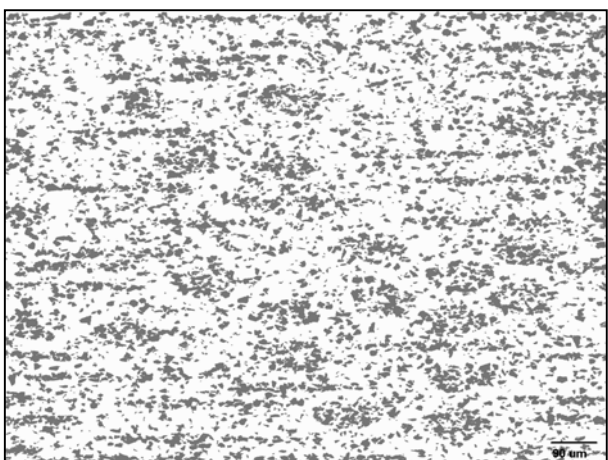


Figure 2: Simulated microstructure

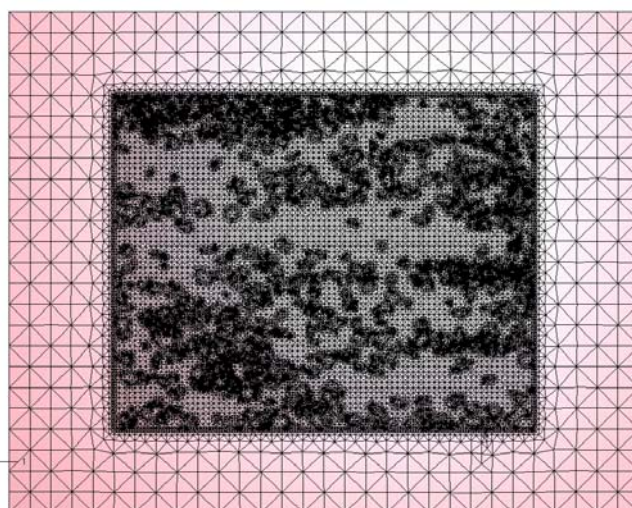


Figure 3: FE Mesh of microstructure

References

- [1] S. Ghosh et al., *Acta Materialia*, 45 (1997) pp. 2215-2234.
- [2] J. Segurado et al., *Acta Materialia*, 51 (2003) pp. 2355-2369.
- [3] Ch. Dietrich et al., *Computational Materials Science* 1 (1993), pp. 195-202.
- [4] J. E. Spowart and D. B. Miracle, *Materials Science and Engineering*, A357 (2003), pp. 111-123.
- [5] S.-J. Hong et al., *Materials Science and Engineering*, A347 (2003), pp. 198-204.
- [6] A. Slipenyuk et al., *Materials Science and Engineering*, A381 (2004), pp. 165-170.
- [7] Acknowledgement: The U.S. National Science Foundation (grant DMR-0404668) and the Air Force Office of Scientific Research (grants F49620-01-1-0045 and 04-NA-152) supported this work. The financial support is gratefully acknowledged.