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14. ABSTRACT
High-resolution large-volume segments of three-dimensional microstructures of a set of boron modified Ti-alloys containing TiB whiskers have been reconstructed and visualized using montage serial sectioning. These microstructures have been quantitatively characterized in detail using stereology and digital image analysis. A novel methodology has been developed for computer simulations of realistic two-dimensional (2D) and three-dimensional (3D) two-phase microstructures where the features have realistic complex shapes/morphologies, spatial clustering, morphological anisotropy, and global microstructural properties statistically similar to those in the corresponding real microstructures. The methodology was applied for simulations of realistic 2D and 3D microstructures of a set of discontinuously reinforced Al-alloy (DRA) composites containing SiC particles of complex shapes and different degrees of spatial clustering, and microstructures of a set of boron modified Ti-alloys having different degrees of morphological anisotropy of the TiB whiskers. Large windows of real and simulated 2D and 3D microstructures have been implemented as representative volume elements in the finite elements based frameworks to simulate the mechanical response.

15. SUBJECT TERMS
Microstructure characterization, microstructure simulations, DRA composites, boron modified titanium alloys

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   Arun M Gokhale

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   Dr. Joan Fuller

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8. **Annual Accomplishments (200 words maximum):**

   High-resolution large-volume segments of three-dimensional microstructures of a set of boron modified Ti-alloys containing TiB whiskers have been reconstructed and visualized using montage serial sectioning. These microstructures have been quantitatively characterized in detail using stereology and digital image analysis. A novel methodology has been developed for computer simulations of realistic two-dimensional (2D) and three-dimensional (3D) two-phase microstructures where the features have realistic complex shapes/morphologies, spatial clustering, morphological anisotropy, and global microstrucutral properties statistically similar to those in the corresponding real microstructures. Using this methodology, virtual microstructures can be simulated for any specified two-point correlation functions, volume fractions, and size distributions of the two phases. The methodology was applied for simulations of realistic 2D and 3D microstructures of a set of discontinuously reinforced Al-alloy (DRA) composites containing SiC particles of complex shapes and different degrees of spatial clustering, and microstructures of a set of boron modified Ti-alloys having different degrees of morphological anisotropy of the TiB whiskers. Large windows of real and simulated 2D and 3D microstructures have been implemented as representative volume elements (RVEs) in the finite elements based frameworks to simulate the mechanical response. The methodologies developed in this research program provide useful tools for simulations based materials design.

9. Archival Publications (published) during reporting period:

1. A.M. Gokhale, H. Singh, and Z. Shan: "Microstructure Representation and Simulation Tools for Microstructure-Based Computational Micro-Mechanics of Heterogeneous Materials," Computational Methods, eds., G. R. Liu, V. B. C. Tan, and X. Han, Springer, Netherlands, Vol. 2, PP 1629-1633, 2005.
2. A. Sreeranganathan, H. Singh, and A.M. Gokhale: "Finite Element Based Modeling of Micromechanical Response of Computer Simulated Realistic Microstructures," Computational Methods and Experiments in Materials Characterization II, eds. C.A. Brebbia and A. A. Mammoli, WIT Press, Boston, PP 291-300, 2005.
3. H. Singh, Y. Mao, and A.M. Gokhale: "Application of Digital Image Processing for Implementation of Complex Realistic Particle Shapes/Morphologies in Computer Simulated Heterogeneous Microstructures," Modeling and Simulations in Materials Science and Engineering, Vol. 14, PP 351-363, 2006.
4. H. Singh, A.M. Gokhale, Y. Mao, and J. E. Spowart: "Computer Simulations of Realistic Microstructures of Discontinuously Reinforced Aluminum Alloy (DRA) Composites", Acta Materialia, Vol. 54, Issue 8, PP 2131-2143, 2006.
5. S. I. Lieberman and A.M. Gokhale, "Reconstruction and Visualization of Three-Dimensional Microstructure of TiB Whiskers in an Extruded Ti-6Al-4V-B Alloy," Scripta Materialia, Vol. 55, PP 63-68, 2006.
6. A M Gokhale, H Singh, Y Mao, A Sreeranganathan, S I Lieberman, S G Lee, "Computer Simulations of "Realistic" Microstructures for Materials Design And Development," Proceedings of International Conference on Recent Advances in Materials and Processing: RAMP-2006, Coimbatore, India, P. C. Angelo, eds., PSG College of Technology, Coimbatore, India, 2006, Section 2.1, PP 1-7 (CD).
7. A. Tewari and A.M. Gokhale: "Computations of Contact Distributions for Representation of Microstructural Clustering," Computational Materials Science, Vol. 38, PP 75-82, 2006.
8. Arun M Gokhale, Harpreet Singh, Scott I Lieberman, and S. Tamirisakandala: "Simulations of Microstructural Geometry for Materials Design," Proceedings of Twelfth International Conference on Plasticity and its Current Applications, Halifax, Canada, July 17-22, 2006, Edited by A. Khan and R. Kazmi, NEAT Press Inc., Baltimore, MD, PP 262-264, 2006 (CD).
9. S. I. Lieberman, H. Singh, Y. Mao, A. Sreeranganathan, A. M. Gokhale, S. Tamirisakandala, and D. B. Miracle, "Characterization and Simulation of Microstructures of TiB Whiskers in Titanium Alloys Modified with Boron," Journal of Metals, Vol. 59, No. 1, PP 59-63, 2007.
10. Mao, H. Singh, and A. M. Gokhale: "Simulations of Realistic Three-Dimensional Microstructures for Materials Design," Proceedings of 13th International Conference on Plasticity ad its Current Applications: Plasticity 07, A. S. Khan and B. Farrokh, eds, NEAT Press Inc., Baltimore, Chapter 1, PP 10-12, 2007 (CD).
11. S. I. Lieberman, A. M. Gokhale, and S. Tamirisakandala: "Reconstruction of Three-Dimensional Microstructures of TiB Whiskers in Ti-6Al-4V-1B Alloys," Materials Characterization, Vol. 58, PP 527-533, 2007.
12. A. Sreeranganathan, S. I. Lieberman, H. Singh, A. M. Gokhale, and S. Tamirisakandala: "Realistic Micromechanical Modeling and Simulation of Boron Modified Titanium Alloys," Users' Proceedings of 2007 ABAQUS Conference, Paris, France, May 22-24, 2007, published by ABAQUS Inc. PP 546-558, 2007
13. A. Sreeranganathan, A.M. Gokhale, and S. Tamirisakandala: "Determination of Local Constitutive Properties of Ti-Alloy Matrix in Boron-Modified Ti-Alloys Using Spherical Indentation." Scripta Materialia, Vol. 58, PP 114-117, 2008.
14. H. Singh, A. M. Gokhale, S. I. Lieberman, and S. Tamirisakandala: "Image Based Computations of Lineal Path Probability Distributions for Microstructure Representation," Materials Science and Engineering, Vol. 474, no. 1-2, PP 104-111, 2008.
15. H. Singh, A.M. Gokhale, Y. Mao, S. I. Lieberman, S. Tamirisakandala: "Computer Simulations of "Realistic" Partially Anisotropic Microstructures," Computational Materials Science, in press.
16. Y. Mao, A.M. Gokhale, H. Singh, and J. E. Spowart: "Computer Simulations of Realistic Three Dimensional Microstructures Containing Complex Realistic Three-Dimensional Particle Shapes and Morphologies," Computational Materials Science, Submitted.
17. S. I. Lieberman, A.M. Gokhale, S. Tamirisakandala, and R. B. Bhat: "Three-Dimensional Microstrucutral Characterization of Discontinuously Reinforced Ti64-TiB Composites Produced Via Blended Elemental Powder Metallurgy," Materials Characterization, Submitted.

10. Changes in research objectives (if any):

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11. Change in AFOSR program manager, if any:

12. Extensions granted or milestones slipped, if any:

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13. Attach Final Report (max. 2MB)(If the report is larger than 2MB, please email file to program manager.)

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