Multi-Scale Modeling, Simulations and Experiments of Coating Growth on Nanofibers

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Overview of Current Investigations

The coating of nanoscale structures and the evolution of crystalline structure at the nanoscale are and will continue to be important issues. Our efforts in this area include a coordinated experimental and modeling program for the synthesis of core/clad and hollow nanowire structures. Physical vapor deposition techniques are used to apply coatings to electrospun polymer nanofibers. These fibers are coated with films of copper, aluminum, titanium, zirconium and aluminum nitride by using a plasma enhanced physical vapor deposition (PEPVD) sputtering process.

To aid the understanding of the deposition process on nanoscale size structures, a comprehensive model for the coating of nanofibers within a traditional PEPVD system has been developed. The model integrates across atomic to continuum length scales for simulating the sputtering, transport and deposition of coating material onto a nanoscale substrate. The model connects macroscale phenomena to nanoscale phenomena by linking simple models at each length scale. The solution procedure involves many simplifying assumptions to piece together a collection of simple models into one comprehensive model. Solution strategies that couple continuum and atomistic models are used. Information is passed between the various length scale models so that the simulations are integrated together. To keep the numerical simulations at a manageable

level, asymptotic analyses are used to reduce the complex models to simpler, but still relevant, models.

Publications

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3. "Development of Experimental Techniques and an Analytical Model for Aluminum Nitriding", R. Evans, A. Salifu, G. Zhang, E. Evans, S. I. Hariharan and G. W. Young, *Surface and Coatings Technology*, Vol. 157 (2002), pp. 59-65.

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   This paper was selected for the Nanotech Virtual Showcase at the Nanotech 2004 Conference and Tradeshow and for Nanopolis - The Distributed Knowledge Network for Nanoscale Science and Engineering. The Nanotech Virtual Showcase featured the best papers of the conference through multimedia animations representing their central concept.

5. "Multi-Scale Modeling, Simulations and Experiments of Coating Growth on Nanofibers: Part I - Sputtering", A. Buldum, I. Busuladzic, C. B. Clemons, L. H. Dill, K. L. Kreider, G. W. Young, E. A. Evans, G. Zhang, S. I. Hariharan, and W. Keifer, *J. Applied Physics*, Vol. 98, (2005), pp. 044303-044303-10.

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of links to articles from participating publishers, covering a focused area of frontier research.

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10. "Modeling and Simulation of Coating Growth on Nanofibers", J. Wilder, C.B. Clemons, K.L. Kreider, G.W. Young, E. Evans and G. Zhang, *J. Applied Physics*, Vol. 105 (2009), pp. 0543171-0543178.

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2. NASA Glenn Cooperative Agreement for Theory, Modeling, Software and Hardware Development in Computational Materials Science - NASA Grant No. NCC 3-1094, (2003 – 2004) $64,000, G. W. Young – PI, C. B. Clemons and S. I. Hariharan.

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4. NSF DMI - “NIRT: Nanofiber Manufacturing for Energy Conversion and Utilization” NSF Grant No. DMI-0403835, (2004 - 2008): $1,300,000, D. Reneker - PI, G. Chase, E. Evans, D. Smith, R. Ramsier, A. Buldum, S. I. Hariharan, K. Kreider, G. W. Young and A. Yarin.