Division of Materials Science and Engineering
Office of Basic Energy Sciences
US Department of Energy

1. DOE award # and name of the recipient (Institution)

DOE-FG02-06ER46289
Rutgers University

2. Project Title and name of the PI

Mesoscale Interfacial Dynamics in Magnetoelectric Nanocomposites
Three Years' Report
Armen G. Khachaturyan (PI)

3. Date of the report and period covered by the report

August 06 2009
August, 2006 – August, 2009

4. Brief Description of accomplishment. This can be in bullet form or whatever you think is useful and appropriate to indicate the sense of progress. Please limit the section to no more than 5 pages

(i) Theory and modeling of chessboard-like self-assembling of vertically aligned columnar nanostructures in films has been developed. By means of modeling and three-dimensional computational simulations, we proposed a novel self-assembly process that can produce good chessboard nanostructure architectures through a pseudo-spinodal decomposition of an epitaxial film under optimal thermodynamic and crystallographic conditions (appropriate choice of the temperature, composition of the film, and crystal lattice parameters of the film and substrate). These conditions are formulated. The obtained results have been published on *Nano Letters*.

(ii) Based on the principles of the formation of chessboard nanostructured films, we are currently trying to find good decomposing material systems that satisfy the optimal conditions to produce the chessboard nanostructure architecture. In addition we are under way doing "computer experiments" to look for the appropriate materials with the chessboard columnar nanostructures, as a potential candidate for engineering of optical devices, high-efficiency multiferroics, and high-density magnetic perpendicular recording media. We are also currently to investigate the magnetoelectric response of multiferroic chessboard nanostructures under applied electric/magnetic fields.

(iii) A unified 3-dimensional phase field theory of the strain-mediated magnetoelectric effect in magnetoelectric composites is developed. The theory is based on the established equivalency paradigm: we proved that by using a variational priciple the exact values of the electric, magnetic and strain fields in a magnetoelectric composite of arbitrary morphology and their coupled magneto-electric-mechanical response can be evaluated by considering an *equivalent* homogeneous system with the specially chosen effective eigenstrain, polarization and magnetization. These equivalency parameters are spatially inhomogeneous fields, which are obtained by solving the time-dependent Ginzburg-Landau equations. The paper summarizing these results is to be submitted to JAP. We are currently using the computational model based on the unified phase field theory to predict the local and overall response of the magnetoelectric composites with arbitrary configuration under applied fields, and to find the optimal composite microstructure that produces the strongest ME coupling.

(iv) We have developed modeling and simulations to support Dr. S. Pryia efforts to produce the strongest ME coupling by searching the optimal configuration of applied electric/magnetic fields, and microstructure of polycrystalline multiferroics. An analytical model demonstrates that the optimization of a magnetoelectric (ME) coupling of a laminar magnetic/piezoelectric polycrystalline composite could be obtained by a proper choice of the magnetic and electric poling directions and the directions of the applied a.c. fields. The results have been published on JAP. Our next step is to determine the domain of optimal parameters and configurations by using our optimization theory and computational modeling.

5. A list of papers (already published, in press, submitted) in which DOE support is acknowledged.

Journal papers

1. Y. Ni, A.G.Khachaturyan, "Phase field approach for strain-induced magnetoelectric effect in multiferroic composites" Journal of Applied Physics, 102, 113506 (2007).
2. R.A. Islam, Y. Ni, A.G. Khachaturyan, S. Priya, "Giant magnetoelectric effect in multilayered composite structures", Journal Applied Physics 104 044103 (2008).
3. Y. Ni, S. Priya, A.G. Khachaturyan, "Modeling of magnetoelectric effect in polycrystalline multiferroic laminates influenced by the orientations of applied electric/magnetic fields", Journal Applied Physics 105 083914 (2009).
4. Y. Ni, W. F. Rao, A.G. Khachaturyan, "Pseudo-spinodal mode of decomposition in films and formation of chessboard-like nanostructure", Nano Letters, published on-line, http://pubs.acs.org/doi/abs/10.1021/nl901551j. (2009).
5. Y. Ni, A.G. Khachaturyan, "Phase field modeling of magnetoelectroelastic solids with arbitrary inhomogeneities", being submitted,(2009).

Conferences

1. Y. Ni, A.G. Khachaturyan, "Phase field modeling of multiferoic composites", MS&T'08, Pittsburgh, Pennsylvania, USA. (oral presentation)
2. Y. Ni, A.G. Khachaturyan, "Origin of the nano-chessboard structures: from tweed to two-phase chessboard architecture", MS&T'08, Pittsburgh, Pennsylvania, USA. (invited talk)

6. A list of people working on the project –graduate students, postdocs, visitors, technicians, etc. Indicate for each whether receiving full or partial support. In case of partial support indicate percentage of support.

Professor A. G. Khachaturyan, co-PI,
Dr. Yong Ni, Research Associate. Dr. Ni has a partial support (20 %).

7. Planned activities for next year, which could be a short paragraph.
We will put forward our joint efforts with Drs. S. Pryia and D. Viehland to grow films with a good regular multiferroic Chessboard nanowire structure. Based on our new theory of chessboard-like self-assemblage of nanowires, we expect to find the optimum processing requirements for $BaTiO_3$-$CoFe_2O_4$ and other systems.

8. An update list of other support (current and pending, federal and non-federal.) For each, indicate the overlap, if any, and/or distinctiveness with the DOE supported project. This could be brief – one or two sentences.
Project title: **Thermodynamics and Kinetics of Structural Transformations in Metal and Ceramic Systems**
1. Support: Current
Project title: **Structural Magnetostrictive Alloys: New Materials for Revolutionary Transducers and Adaptive Engineered Systems**
Source of support: ONR (MURI proposal) grant N00014-06-1-0530
Total award: $241,810 (220459+21351=$ 241810)
Period covered: 05/01/2006 – 12/31/2009
Location of Project: Iowa State Univ., Ohio State Univ., Penn. State Univ.,
Rutgers Univ., Univ. of Minnesota and Virginia Tech
Rutgers University, Department of Materials Science and Engineering
Person-Months per Year Committed to the Project. Cal: 0.00. Sumr: 1
Project title: **Thermodynamics and Kinetics of Phase Transformations in Complex Non-Equilibrium Systems**
Source of support: NSF, DMR, Materials Theory, 0704045
Total award: $127,000×3=$381,000
Period covered: 09/01/2007 – 08/31/2010
Location of Project: Rutgers University, Department of Materials Science and Engineering
Person-Months per Year Committed to the Project. Cal: 0.00. Sumr: 1

9. Cost status: Show approved budget by the budget period, actual costs incurred by the date of the report and projected unspent funds at the end of the current budget period. If any cost-sharing is required, breakout by DOE share, recipient share and total costs.
Total budget for 08/01/2006~07/31/2009: $50,014×3
Actual cost at the date of report $62,629
Projected cost at the end of the budget period $13,850
Balance at the end of the budget period will be $4000-the partial support of Dr. Ni will be increase to 28% from 20% now.

Previously the partial support is 20%, now if we change the balance from 12000 to 4000, there is another 8000 to be used to increase Yong Ni's support. And the increased percentage is 8000/(1+0.325+0.545)/51000=8%. Therefore the partial support of Dr. Ni will be increase to 28% from 20% now.