Minutes of kick-off FRG meeting:
When: March 15, 2000
Where: Nashville, Tennessee (TMS meeting)
Who: Armen Khachaturyan, David Laughlin and Yunzhi Wang

Discussed the starting date of the project, hiring of graduate students and postdoc fellows, and the starting system and focusing issues.

1) David raised a concern about the hiring of graduate students. It may have some difficulty to find the students that we need before the summer. It should be much easier if the project starts in the Summer. Yunzhi will contact OSU financial administration person or NSF for possibilities.
2) It will be ideal if David can convert his student in the budget into a postdoc, considering the fact that the cost is almost the same.
3) David will seek the opportunity to use the Japanese ultra-high voltage TEM, in which stress can be applied in-situ.
4) David would like to have a recommendation letter from the instructor of the TEM course that the postdoc candidate (Andrei Kanzaruan) is taking.
5) David will write a short description of the significance of the project, including some details on the system that we will start with, what are the experimental observations of the system in terms of crystal structures, domain morphologies and phase transformation mechanisms, the critical issues in terms of microstructural engineering and how the simulations can help. Then Armen and Yunzhi can (1) start to formulate the model, develop numerical method and algorithms; (2) searching for good graduate students.
6) Armen would like to either pay a visiting professor who is working with him on on-going project using parallel codes or transfer his student in the budget to OSU if he cannot find a good student at Rutgers. Yunzhi will find out the procedures for the transfer.
7) David recommended that we should start with Fe-Pt or Co-Pt, thin film deposited on a substrate with epitaxial stress, single crystal first and then extended to polycrystalline system. The as-sputtered film is a disordered FCC phase which will transform into ordered domains. The interesting things to look at are the formation of the ordered domains in the absent and present of an applied stress. For magnetic recording media, it is desirable to have the c-axes randomly oriented in the plane of the film.

Minutes of phone meeting with David Laughlin
When: June 8, 2000

Three overall research thrusts for the project suggested by David (please correct me if I am wrong):

1) Single Crystal Epitaxy: epitaxial thin film deposited on single crystal substrate. The as- deposited film is single crystal fcc (A1) phase (but ferromagnetic) and transforms into $L1_0$ during aging. The A1 → $L1_0$ congruent transformation mechanism could be either nucleation and growth, or continuous ordering. The epitaxial stress could be in tension or compression. I assume the [100] direction of the film is pointing up. The key issues involved include:
   - Congruent ordering under epitaxial stress (biaxial stress), nucleation and growth of the $L1_0$ phase out of fcc phase. Final state: single phase of $L1_0$.
   - How to align the c-axis of the three orientation variants of the $L1_0$ phase to get either longitudinal or perpendicular c-axis in the film, by applying magnetic field and/or control the epitaxial stress
   - If the c-axis is either longitudinal, then how does the ordered domain (polytwin structure) control the magnetic domain, e.g., how does the boundaries between two microtwin plates interact with the magnetic domain walls and contributes to the domain walls pinning. If the c-axis is perpendicular, then there is no polytwin structure and no twin boundary pinning. What will be the coercivity? Higher or lower?

2) Polycrystalline Epitaxy Thin Film: In the as-deposited film, the <100> axis of all the fcc grains pointing up (perpendicular to the film), forming a fiber texture. The other two cubic axes are randomly oriented in the plane of the film. Grain boundaries could be high angle or low angle. There is no grain growth problem in the heat treatment. The as-deposited grain size is about 20nm and does not change much during the subsequent heat treatment. Within each grain, it is either a single variant, or several variants but without forming the polytwin assembly. During the heat treatment, the fcc phase transforms into $L1_0$ phase through either nucleation and growth (starting from grain boundaries) or continuous ordering. The key issues involved include:
   1) Ordering reaction within each grain under epitaxial stress
   2) Ordering reaction within each grain under epitaxial stress and applied magnetic field. How to align the c-axes of the grains either perpendicular to the plane of the film or in the plane.
   3) Effect of grain boundary on the coercivity of the film.
   4) The coercivity of single variant grain vs. the coercivity of multi-variant grains.

3) Same as 2) but the <111> axes of all the grains in the as-deposited fcc film pointing up. Commercially it may be less important but it could be interesting to study because in this case, the c-axes are either in or perpendicular to the plane of the film. The ordering reaction under epitaxial stress and applied magnetic field and the subsequent domain switching under external magnetic field may be quite different.

According to these processes, Yunzhi and Armen will meet at Rutgers on June 14 through 16 to discuss the challenges to mathematical modeling and computer simulation. Phone calls to David are anticipated if some details come up which need clarifications.

Minutes of meeting on November 30, 2000 (MRS meeting)
When: November 30, 2000
Where: Boston (MRS meeting)
Who: Armen Khachaturyan, Yunzhi Wang, Andrei Kazaryan, Youhai Wen and YongMei Jin

Reported and discussed of the simulation work on different hierarchy of the ploytwin type structural and magnetic domain structures.

Reported and discussed the simulations results on polycrystalline thin films

Discussed new formulation of the governing equations to handle more efficiently the boundary conditions.

Minutes of Semi-Annual Meeting
When: 02/08/01
Where: Carnegie Melon University
Who: Armen Khachaturyan, David Laughlin, Yunzhi Wang, Andrei Kazaryan and Lisha Wang

Presented both experimental and simulation work of the projects.
Discussed future direction of the research.

Minutes of meeting at Rutgers, February 27 – 28, 2001

1) Discussed the results obtained for magnetic structures in 3-D polytwin systems with fixed microstructure. Results are compared with the existing experimental observations of magnetic structure in hard ferromagnetic materials like *Fe-Pt* and *Fe-Pt*. This contains hierarchy of magnetic domains in single twins, colonies and packets. Similarly to experimentally observed structures, results of computer simulations indicate that only packets of twin plates can be considered as magnetically independent units. Ways to optimize computer simulations are discussed as well, by utilizing the fact that colonies of twins can be considered as uniaxial ferromagnets with the easy axis in the average magnetization direction of two adjoining twins. Taking this into account only slightly changes the model, however allows to consider much larger system sizes.
2) Application of external fields and calculation of hysteresis loops is discussed. Simulation of magnetization reversal requires introduction of free surface or other structural defects. This will make possible for nucleation and subsequent motion of magnetic macro-domain walls in the presence of externally applied magnetic fields.

3) Details of computational code for efficient parallelization and usage of multiprocessor computers (T3E) were discussed.

Minutes of meeting at Rutgers, June 14 – 16, 2001

1) Discussed model formulation and technical challenges
2) Since the order – disorder transformation temperature is much higher than the Curie temperature (need to be confirmed), we will start the simulation with single crystal /polycrystal thin films of existing microstructure. We can start with any microstructure and investigate its impact on magnetic properties. In the simulations, what we need to do is to solve the time dependent phase field equations for M and leave the kinetic equation for the long-range order parameter out. This means that the underlying starting microstructure will be frozen during the evolution of the magnetic domain w/o applied magnetic field. Andrei will start with single crystal and Yong-Mei will start with polycrystalline film. However, if we have a fixed initial microstructure and assume a single grain is a single tetragonal L10 domain, then the simulation will be pretty much the same for the polycrystalline and single crystal, with different number of lro parameters characterizing the starting microstructure.
3) After the models are developed and tested, parameters of real system will be used for productive runs and the simulation results will be reported to Prof. Laughlin for validation.
4) Transformation of fcc – L10 under epitaxial stress. We need to handle the heterogeneous stress state associated with the heterogeneous microstructure in the film and new theoretical model/approximation need to be developed.
5) Our first Annual Report is due on Jan. 1, 2001. I propose a meeting at the MRS meeting to have all the results exchanged and to have the Report outlined. Then each of us will fill in the details and I will put everything together.