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Subject: Final Performance Report

Grant Title: The Effective Behavior of Heterogeneous Ferromagnetic Materials

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In the project, we have studied a variety of heterogeneous ferromagnetic materials, including ferromagnetic shape memory alloys, multiferroic materials, and ferromagnetic composites. The main achievements have been summarized as following:

1. A constrained theory of magnetoelastic materials has been developed to study the effective behavior of single-crystalline and polycrystalline ferromagnetic shape memory alloys (FSMA) based on nonlinear homogenization theory and variational principle. The actuation strain induced by domain switching under a combined magneto-mechanical loading has been established first for single crystalline FSMA, from which the strain in FSMA polycrystals has been derived using Taylor estimate. Both NiMnGa and FePd have been analyzed, and the necessary fiber textures for large actuation strain in FSMA polycrystals have been identified. It was discovered that both twin boundary motions and magnetization rotations contribute to the magnetic field induced strain, but the twin boundary motions are blocked when the compressive stress exceeds a critical values, leading to substantially smaller magnetic field induced strain and thus relative low blocking stress.

2. An unconventional phase-field theory has also been developed to study the microstructural evolution and the macroscopic properties of ferromagnetic shape memory alloys (FSMA) based on nonlinear homogenization theory and variational principle. The theory has been systematically implemented into numerical simulations to study the effective behavior of FSMA under the combined mechanical and magnetic loading. It is discovered that while both twin boundary motions and magnetization rotations contribute to the magnetic field induced strain, the twin boundary motions are blocked when the compressive stress exceeds a critical values, leading to substantially smaller magnetic field induced strain and thus relative low blocking stress. This confirms our earlier theoretical analysis based on the constrained theory, and the numerical simulations agree well with experimental observations.

3. A continuum theory has also been developed to describe the antiferromagnetic coupling among magnetic spins, and has been incorporated in the phenomenological theory of multiferroic materials for phase-field simulation. The method has been implemented to investigate the magnetoelectric domains in multiferroic bismuth ferrite, wherein ferroelastic, ferroelectric, and antiferromagnetic orderings coexist in the single-phase material at room temperature. The magnetoelectric domains have been simulated for the first time, and the manipulation of magnetic domains by electric field has also been

demonstrated, in excellent agreement with experimental observations. In addition, the switching of magnetic domains by mechanical stress has been also predicted.

4. Bulk magnetic composites consisting of hard matrix and soft second-phase fillers have also been analyzed using effective medium theory, with the objective to understand the unusual experimental observation of energy product enhancement in composites with large second-phase fillers, where exchange coupling is negligible. The analysis demonstrates that the enhancement is resulted from the magnetostatic interactions among magnetic grains.