

Structure-Sensitive Properties of Advanced Permanent Magnet Materials: Experiment and Theory

Description: This program, a joint endeavor of BNL and INEEL, elucidates the relationships linking the microstructure of advanced permanent magnetic materials to their magnetic properties, with the ultimate goal of understanding how the microstructure may be manipulated and organized into desirable microstructures by suitable processing methods. The research has focused on the effects of lattice defects (*e.g.*, grain boundaries, secondary phases, degree of crystallinity and nonstoichiometry) upon hysteretic properties in prototypical rare-earth-based intermetallic compounds such as Nd₂Fe₁₄B and SmCo₅. Special attention has been paid to the effects of non-equilibrium processing methods such as rapid solidification achieved by melt-spinning or gas atomization.

Program Highlights: Optimization of Permanent Magnets Processing:

- The effective quench rate of gas-atomized Nd₂Fe₁₄B-based powders is increased when processed with the elemental additives Ti and C. This addition results in a glassy microstructure amenable to magnetic property optimization.
- Bulk transmission x-ray diffraction performed at the NSLS on thermomechanically-deformed melt-quenched Nd₂Fe₁₄B-based magnets have quantified texture as a function of position, deformation level and have provided recommendations for process improvement.
- Theoretical estimation of the thermodynamic properties of point defects, non-stoichiometry, and phase transitions in SMC05+x and Sm₂CO_{17-y}; such results are expected to assist in the optimization of rapid solidification processing of these materials.

Elucidation of Role of Exchange Interactions in Magnetic Reversal, Magnetic Properties:

Quantitative high-resolution transmission electron microscopy coupled with magnetic measurement have revealed the dominance of exchange interaction in the reversal behavior of nano-scaled permanent magnets. Curie temperatures of the Nd₂Fe₁₄B phase in Nd₂Fe₁₄B/a-Fe exchange-coupled nanocomposites increase with increasing excess iron; such effects are tentatively attributed to interphase exchange coupling and may have important consequences concerning the operating temperature of such magnets.

Impact: The early emphasis that we placed on the importance of intergranular exchange coupling on the magnetic properties of pertinent nanoscaled magnetic materials has superseded the previous widely-held notion that short-range interactions were negligible in these materials. Such concepts provide increased understanding of the magnetic properties of these compounds and guiding principles for their improvement. Discovery of the microstructural control via selected alloying additions in rapidly-solidified Nd₂Fe₁₄B-based alloys has resulted in significant industrial interest and investment as well as one spin-off company, GA Powders, Inc. Despite its youth, the BNL program continues to gain significant respect in the field. An outgrowth of this good reputation is that we receive frequent inquiries from faculty and graduating students from top universities in the field, as well as from many industrial representatives, concerning the possibility of collaborative work and joint proposals.

Interactions:

The program features a large number of research collaborations, which have helped to forge links between scientific laboratorybased understanding and practical field-based results, thus facilitating the transformation of basic knowledge to the applied sector. *National Laboratory Collaborations:* Ames Lab (fundamental studies of solidification in melt-spun Nd₂Fe₁₄B, hysteresis

loop modeling), LBL (electron microscopy of thermomechanically-deformed magnets);

Academic Collaborations: Lehigh University (reversal studies in model thin film systems), Carnegie Mellon University (cc"-Fe₁₀₂, high-temperature permanent magnets), Queens College-CUNY (many-atom potential models of cohesion in intermetallic compounds), University of Utah (electron microscopy);

Industrial Collaborations: Magnequench International, Inc. (general structure/property interrelationships in Nd₂Fe₁₄B-based magnets), Rh6ne-Poulenc/Rhodia, Inc. (microstructural evolution in exchange-coupled nanocomposites), IAP Research, Inc. (deformation of Sm-Co magnets).

Personnel:

D. J. Branagan (INEEL, experimental studies), L. H. Lewis (BNL, experimental studies), C. H. Sellers (INEEL, experimental studies), D. O. Welch (BNL, theoretical studies), Y. Zhu (BNL, electron microscopy), J.-Y. Wang (BNL, post-doctoral associate), D. Crew (BNL, post-doctoral associate).

Recognition:

- One R&D 100 award
- Two Lockheed-Martin LEAP awards
- BES 1996 Materials Sciences Award
- Three patents
- Eight invited presentations
- Symposium organizer, 1999 Spring MRS Meeting: "Hard Magnets: Principles, Materials, Processing"

Budget: FY 1998: \$488K total; \$378K BNL and \$1 IOK INEEL