Influence of Crystal Chemistry on Magnetoelastic Properties in Fe-Ga Alloys

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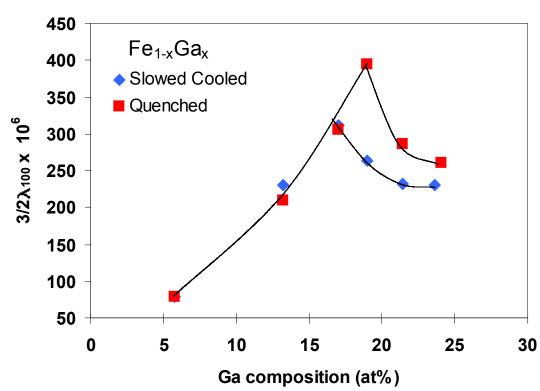
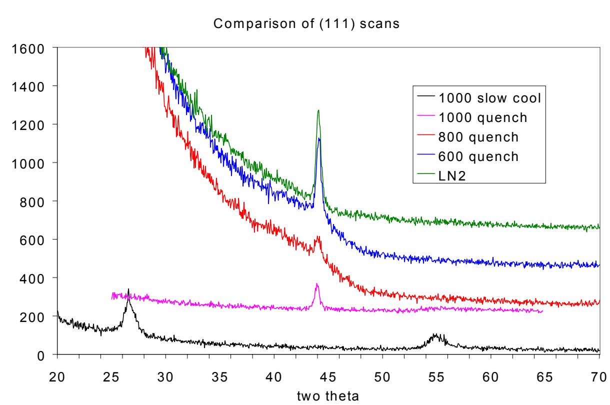
Abstract:

This project is concerned with the structural characterization of alloy systems that exhibit extraordinary magneto-responsiveness in regions of phase and/or structural instabilities. The main goal is to investigate the local atomic structure and structural defects in these critical systems and to analytically correlate these structural aspects to the observed magnetic responses. Research is initially focused on the anomalous increase in magnetostrictive response from ferromagnetic shape memory alloys where large field-induced strains can be achieved and from Fe-based solid solutions with non-magnetic solutes (Ga, Al). In both systems, anomalous magnetic response occurs at specific points within temperature-composition regimes where energy differences between magnetic and crystalline states (chemical ordering, phase transitions, etc.) are similar.

Recent Results:

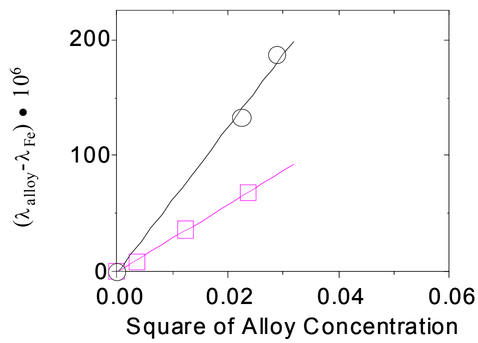
It has recently been found that a substantial increase (20x) in the magnetostriction, (3/2) λ_{100}, of Fe occurs with the substitution of small amounts of Ga for Fe. This is quite a remarkable result given that Ga is non-magnetic. The magnetostriction increases up to 17 atomic % Ga independent of the thermal history, suggesting that enhanced magnetostriction is dependent on maintaining the body-centered cubic (BCC) α-Fe structure and results from local short range ordering of the Ga atoms along specific crystallographic directions in the disordered Fe structure. This is most evident at compositions greater than 17%, where thermal treatment greatly affects the magnetostriction. X-ray diffraction spectra taken from oriented single crystalline samples of Fe-19 at% Ga alloy for different heat treatments have verified that slow cooling results in the formation of DO_3 long range ordering that accounts for the decrease in observed magnetostriction. The isothermal and quenching treatments were found to be successful in preventing the formation of DO_3 as evidenced by the loss of the superlattice peaks regardless of the annealing temperature. However, these treatments did result in the formation of an extra diffraction peak at 2θ ~ 44.0° in both orientations. This extra peak can be indexed to a tetragonal structure based on Cu_3Ti, implying a BCC-FCT transformation has occurred. The FCT structure is layered with the Ga atoms aligned along the parent (100) crystallographic directions.





Significance:

It has been proposed that the many-fold increase in magnetostriction above that of Fe occurs as the BCC lattice is strained along [100] directions due to the emergence of directional short-range order of Ga atoms. This behavior can be understood as being due to the presence of clusters of solute (Ga or Al) atoms which act as both elastic and magnetoelastic defects in the alloy. A simple thermodynamic model predicts that at small concentrations, the saturation strain should increase with the number of Ga–Ga or Al–Al pairs, i.e., as x^2, where x is the amount of Al or Ga. For larger x, it becomes impossible to form the disordered BCC structure, as the alloys partially or fully order into a DO_3 structure. In this larger concentration range, very few clusters can act as magnetoelastic centers. Instead, the magnetostriction falls to a value characteristic of the ordered alloy. Measurements of λ_{111} vs. x, for either $Fe_{1-x}Ga_x$ or $Fe_{1-x}Al_x$ show little or no increase with x, in contrast to the behavior of λ_{100}. This difference is naturally accounted for by assuming that there can be no near-neighbor pairs of Al or Ga, because of the size differentials between Fe and either Ga or Al. In this case, there is no defect-driven contribution to λ_{111}. The next near neighbors are along [100], which contributes to λ_{100}. These are the "pairs" referred to above. The thermodynamic model is related to the pair model of magnetostriction. Experimental verification of structural changes provides support for the propose magnetostriction model based on Ga-Ga pairing along [100]. From a physical standpoint, the BCC-FCT structural transition is attractive since the transition can be accomplished through a simple martensitic shear. Recent elastic constant measurements by Wuttig (U of Maryland), a softening of the shear modulus $c'=(C_{11}-C_{12})/2$ was observed with increasing Ga concentration. It is likely a lattice instability can be triggered in Fe-Ga if the disordered BCC is retained to low temperatures, which can lead to a displacive transformation responsible for the observed structural changes. In addition, recent FLAPW calculations by R. Wu (California State) indicate the FCT structure is magneto-responsive.



Future Work:

Structural analysis of quenched and annealed Fe-19 at% Ga alloys, in single- and poly-crystalline form, will be continued using X-ray scattering experiments (i.e., diffraction and EXAFS), neutron and magnetic scattering measurements for magnetic structures, and electron microscopy to characterize the local clustering of Ga atoms within the Fe lattice. Structural changes will be correlated with magnetostrictive response. These studies will also be extended to higher compositions where long-range ordering effects on the magnetism can be examined. Due to slow transformation kinetics observed in the Fe-Ga alloys between stable and metastable ordered phases, epitaxial nanophase mixtures can be produced where the length scales are sufficiently small to allow for exchange coupling between phases. The structural and magnetism relationships of these unique structures will be examined.

Interactions:

Processing and development of binary and ternary Fe-based magnetostrictive alloys with reduced magnetic anisotropies will continue in cooperation with A. Clark and M. Wun-Fogle of the Naval Surface Weapons Center. These alloys exhibit modest magnetostriction while processing greater toughness and could be applicable as responsive structural members. In addition, elastic constant measurements and magnetoelastic modeling of these alloys is ongoing with J. Cullen and M. Wuttig at UMD, first principle calculations of magnetostriction as a function of crystal structure with R. Wu, California State University, and magnetomechanical modeling with A. Flatau, Iowa State University.