Anexo 2: Ref: ILL2015/VR

Influence of the microstructure on the martensitic transformation and physical properties in magnetic shape memory alloys

Magnetic shape memory alloys (MSMA) have awakened a great interest in recent years due to their potential as sensors, magneto-mechanical actuators and magnetic refrigeration materials. Their technologically interesting properties, based on its response under applied magnetic field, are linked to the induction of the martensitic transformation (MT) and/or martensite variants reorientation. The microstructure (composition, internal stresses, long range order degree, second phase precipitates and density of defects) has a strong influence on the MT characteristics and its associated effects as the giant magnetoresistance and the magnetocaloric effect. Taking advantage of the mentioned features, the scientific community is making a great effort to develop new nano-micro electro-magneto-mechanical devices based on MSMA systems.

This Ph. D. work is in the framework of a research activity developed by the group "Propiedades Físicas y Aplicaciones de Materiales" of the Physics Department of the Universidad Pública de Navarra (UPNa). This research is focused on the analysis of the influence of the defects on the structural and magnetic properties of the MSMA and consequently the defect configuration that optimizes these properties. The study will be focused on both types of MSMA: ferromagnetic, as the Ni-Mn-Ga compounds, and metamagnetic systems, of formula Ni-Mn-X (X=In, Sn, Sb). The main parameters to study are the effect of a fourth alloying element, the concentration of defects and the state of strains and stresses. A main processing route consisting in the application of thermal and mechanical treatments, ball milling among them, is being used to control the mentioned parameters. As a complementary goal, we propose the study of the MT at nanometric scale by using nanoparticles obtained by ball milling and laser ablation. Both elastic and inelastic neutron scattering play a crucial role in the different steps of this study, namely in the characterization of the crystal and magnetic structures, microstructure, and vibrational density of states in the different phases involved in the MT.

The proposed work has an experimental character and provides a huge experience on different techniques of characterization. The activity of the Ph. D. student should be included in this context and it is centered on the use of elastic and inelastic neutron scattering techniques, although the candidate must also participate in preliminary laboratory work (synthesis, processing and characterization) through different short stays at the host institution (UPNa).

Thus, the work plan of the Ph. D. student organized by neutron techniques:

Task 1. Elastic neutron scattering

Study the influence of microstructure on the MT. Ball milling and thermal treatments are used to modify the microstructure and generate defects as vacancies, dislocations and to induce internal stresses. In each step of the process, the microstructure and the structural and magnetic properties are analyzed by calorimetric, magnetic, X-ray diffraction, electron microscopy and positron annihilation measurements.

Neutron diffraction measurements are carrying out on ball milled and treated samples at different stages with two aims: (i) the study of the kinetics of the MT and the recovery process of the microstructure at moderate temperatures by in situ thermodiffraction measurements, and (ii) the determination of the magnetic structure and its evolution with microstructure. Thus, the precise magnetic and crystal structure including deformations and internal stresses must be determined by neutron diffraction, which is an essential tool in the investigation of this type of compounds due to the contrast provided by neutron radiation for elements with similar atomic number.

-Quaternary Ni-Mn-X-Co (X=In, Sn, Sb) poly and single-crystals to study the influence of Co addition on the magnetism and structure of transforming phases. Neutron powder and single-crystal diffraction combined with polarized neutron diffraction to determine the atomic and magnetic structures of the austenite and martensite.

- Nanoparticles of Ni-Mn-Ga and Ni-Mn-In. Powder neutron diffraction to study the influence of the size reduction on the structure and on the MT.

Task 2. Inelastic neutron scattering

The objective is the determination of the phonon DOS of the phases involved in the MT. Starting from the polycrystalline samples of the four alloys systems, time of flight measurements is being used to measure the DOS, aiming at estimating the vibrational contribution to the specific heat and entropy in both phases at different temperatures. In combination with magnetic and calorimetric measurements, it should allow to estimate the different contributions to the MT entropy: vibrational, magnetic and electronic. In addition, by means of measurements at different temperatures (above and below the Curie temperature), the anharmonicity and magnetoelastic coupling will be studied. The work will be carried out on treated samples to determine the influence of mechanical treatments on the vibrational behavior. Finally, the influence of the size reduction on the vibrational behavior will be analyzed by measuring the nanoparticles obtained by ball milling. In addition, by combining the measured DOS with the simulated neutron-weighted one at the ab initio level (containing the vibrational contributions from the different atomic species) the thermodynamical quantities should be extracted.

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