Intermetallic compounds

4 - 1 − Magnetic behavior and magneto impedance effect in iron based ribbons

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The amorphous alloy ribbons $Fe_{90-x}B_xSi_{10}$ with x = 10, 12.5, 15, 17.5, 20 and 22.5, prepared by the melt spinning technique are studied at room temperature by magnetization (M), AC susceptibility (χ_{ac}) and magnetoimpedance measurements, under finite DC applied fields (H). The DC field dependence (H) of the magnetization, M, of the samples was measured, from -1 to 1 KOe, with a vibrating sample magnetometer. H was applied along the longitudinal direction of the samples. The AC susceptibility of the samples was measured for dc applied magnetic field (H) ranged from -80 to 80 Oe, using the standard ac inductance method. The frequency of the AC modulating field (H_{ac}) was applied in the range 10 to 104 Hz, while its amplitude was maintained at H_{ac} ∼1 Oe. The complex impedance in the samples was measured for DC applied magnetic field (H) from -80 to 80 Oe, via the so-called four-probe technique. H was applied parallel to the ac driving current along the longitudinal direction of the samples. Data were obtained for consecutive H-steps, stabilizing H before each reading. The field was swept at a step of approximately 1 Oe. The frequency of the AC driving current was applied in the range 0.5 to 10 MHz, while its amplitude was kept at 1 mA (rms value).The M vs. H curve exhibits soft magnetic behavior, i.e., the loop is square shaped, having low coercivity. The χ'_{ac} curve decreases monotonically from a maximum at $H = 0$. The amplitude of these peaks displays frequency dependence. Similar characteristics were observed in the imaginary part of the susceptibility. The ribbons exhibit soft magnetic behavior, especially giant magneto-impedance effect, GMI. This behavior is consistent with the field dependences of the magnetization and AC susceptibility.

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4 - 2 − Thermoelectric figure of merit of Zn_4Sb_3 samples grown by mechanical alloying and subsequent sintering

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Zn_4Sb_3 alloys were prepared by mechanical alloying (MA) followed by a sintering process of different duration (0 to 50 hours). Transport properties involving electrical resistivity $\rho(T)$, Seebeck coefficient $S(T)$ and thermal conductivity $\kappa(T)$ were studied in the temperature range between 100 and 290K. The Seebeck coefficient and electrical resistivity increase with the sintering time reaching maximum values close to $350\mu V/K$ and $18m\Omega cm$ respectively. The thermal conductivity decreases with the annealing time up to values less than $1W/K-m$. From $\rho(T)$, $S(T)$ and $\kappa(T)$ data it was possible to determine the thermoelectric power factor (PF) and the dimensionless thermoelectric figure of merit ZT, which reach maximum values close to $25\mu W/K^2-m$ and 0.35, respectively. Additionally, the structural and morphological properties of the obtained samples were studied by powder x-ray diffraction analysis and electron scanning microscopy (SEM), respectively.

4 - 3 − First principles calculation of $L2_1$ + A2 coherent equilibria in the Fe-Al-Ti system

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Fe-Al-based alloys, i.e. alloys which contain either disordered A2 α-(Fe,Al), B2-ordered FeAl or $D0_3$-ordered Fe_3Al as majority phase, have a considerable potential for developing materials for structural applications, but insufficient strength and creep resistance have been identified as obstacles for the use of Fe-Al-based alloys at high temperatures. The addition of a third alloy element offers the possibility to produce strengthening by coherent precipitates. The effect has been observed in the Fe-Al-Ti system where coherent A2+$L2_1$ microstructure forms in the rich iron composition range.

By combining ab initio electron theory and statistical mechanics the ground state and the phase equilibria at finite temperatures of the ternary system Fe-Al-Ti have been investigated. Total energy calculations have been performed by means of the Wien 2k code to stablish the ground state energetics. A cluster expansion method was therewith used to describe solid solutions. At several chosen finite temperatures the Cluster Variation Method in the irregular tetrahedron approximation was employed in order to calculate the iron rich ternary bcc equilibria. It is confirmed that there are two kinds of phase separations of the bcc phase, A2+$L2_1$ and B2+$L2_1$.

4 - 4 – Crystallization Kinetics of Soft Magnetic Amorphous FeBSi Ribbons

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The crystallization kinetics of amorphous soft magnetic ribbons, $Fe_{90-x}B_xSi_10$ with x = 10, 12.5, 15, 17.5, 20 and 22.5, is studied using differential scanning calorimeter (DSC) and thermo-gravimetric analysis (TGA). At low concentrations of boron (10 ¡ x ¡ 15), the DSC profiles show clearly a two-stage crystallization process. For higher concentrations (15 ¡ x ¡ 22.5) only one-stage crystallization process is observed. It suggests that the boron delay the beginning of the nanocrystallization process inside the amorphous matrix. The study of the crystallization kinetics of materials above is of particular interest due that present excellent magnetic property in its amorphous as well as nanocrystalline state, and the crystallization kinetics provide an idea of when these properties begin to deteriorate [1]. The activation energies for crystallization kinetics, Ec, for $Fe_{90-x}B_xSi_{10}$ with x = 10, 12.5, 15, 17.5, 20 and 22.5 have been evaluated from DSC data using different non-isothermal methods derived through Kissinger [2], Avrami [3] and Ozawa [4]. On the other hand, a comparison between DSC and TGA profiles allowed the determination of the primary crystallization temperature, Tp1, and of the amorphous Curie temperature, Tc-am, in these compounds. The influence of the amount of boron on the crystallization kinetics and thermal and magnetic stability of $Fe_{90-x}B_xSi_{10}$ alloys is discussed.

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4 - 5 – U-Al ground state. An ab-initio and many body approach.

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The U-Al binary system exhibits the formation of three intermetallic compounds: cubic Laves phase C15 Al_2U, cubic $L1_2$ Al_3U, and orthorhombic $D1_b$ Al_4U. However, some uncertainties are found in the literature concerning Al_4U structure and composition. A computational first principles based approach is a useful tool to shed some light into this problem. To the authors knowledge there seem to be no such contribution.

Formation energies of the stable structures at zero kelvin as a function of composition, as well as several metastable and unstable structures are calculated in the binary alloy system U-Al by means of the Full Potential Linear Augmented Plane Wave method implemented in the Wien 2k software package. The ground state is obtained in acceptable agreement with experimental determinations. Therewith, a many body interaction potential is fitted to the calculated energy data. The reliability of the potential was tested by analysing relative structures stabilities at fixed compositions. Al_4U stabilization with composition and uranium constitutional vacancies is specially discussed.

4 - 6 – Antiferromagnetic calculations of random γ-FeMn alloy

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The magnetic structure in γ-FeMn alloys has been the subject of numerous studies over the last decades [1-2]. In the study of the antiferromagnetism of γ-FeMn, three models (1Q, 2Q and 3Q) for the spin structure have been proposed [1]. Even the efforts to unambiguously determine the ground state magnetic structure or to exclude one of the three models, some differences on experimental results have been found, keeping some lack in the full description of the system. In this way, neutron diffraction results cannot distinguish between noncollinear 3Q states and a collection of domains individually ordered in a collinear 1Q state [1], Mössbauer spectroscopy results indicate that both, 3Q or 2Q magnetic structures are possible[3], and inelastic neutron scattering supports the 1Q spin model [4]. These discrepancies make this system an interesting candidate to study by ab initio calculations.

Lately, several calculations of the antiferromagnetic γ-FeMn structures have been performed using the ordered L10 structure. These calculi tilted the balance to the 3Q spin state, but this crystallographic structure doesn´t completely represents a random alloy. Regarding that, on this work, preliminary results of the three spin states calculated using a full-potential linearised augmented-plane wave (FP-LAPW) code for a 50-50 random γ-FeMn alloy are presented.

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[4] P. Bianti, G. Mazzone, and F. Sacchetti, J. Phys. F **17**, 1425 (1987).

4 - 7 – The negative electrode development for a Ni-MH battery prototype

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The negative electrode development for a nickel-metal hydride battery (Ni-MH) prototype was performed with the following procedure: 1) the $Lm_{0.95}Ni_{3.8}Co_{0.3}Mn_{0.3}Al_{0.4}$ intermetallic alloy (Lm = lanthanum rich mischmetal) was crushed, sieved between 44 and 74 μm and mixed with teflonized coal; 2) the compound was assembled together with a current collector and pressed in a cylindrical matrix. The obtained electrode presented a disc shape, with 11 mm diameter and approximately 1 mm thickness. The crystalline structure of the hydrogen storage alloy was examined using X-ray diffractometry. The measured hcp lattice volume was 1.78 % greater than the precursor $LaNi_5$ alloy, increasing the available space for hydrogen movement. Electron dispersion spectroscopy (EDS) and scanning electronic microscopy (SEM) measurements were used before and after hydriding in order to verify the sample homogeneity. The negative electrode was electrochemically tested by using a laboratory cell. It almost totally activates in its first cycle, which is an excellent characteristic from the commercial point of view. The maximum discharge capacity reached was 314.2 mAh/g in the 10^{th} cycle.