HYPERFINE INTERACTIONS IN SOLIDS

[1]Carbonari, A.W.; [1]Mestnik-Filho, J.; [1]Saxena, R.N.; [1]Lapolli, A.L.; [1]Domienikan, C.; [1]Junqueira, A.C.; [1]Cavalcante, F.H.M.; [1]Pereira, L.F.D.; [1]Cordeiro, M.R.; [1]Leite, D.M.T.; [1]Mercúrio, M.; [2]Cabrera-Pasca, G.A.; [2]Oliveira, J.R.B.; [2]Rizzutto, M.A.; [2]Rechenberg, H.R.; [3]Saitovitch, H.

[1]Centro do Reator de Pesquisas - IPEN/CNEN-SP; [2]Instituto de Física - USP; [3]Centro Brasileiro de Pesquisas Físicas, CBPF, RJ

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The interactions between the nuclear moments and the extranuclear electromagnetic fields (magnetic fields or the electric field gradient) are called hyperfine interactions. Measurements of these interactions provide a very sensitive and accurate method to investigate condensed matter phenomena in many different solids. A large variety of phenomena in solid materials, in general, originates from small differences in their electronic structure. In this perspective, it is of specific interest to investigate series of compounds where one can vary the constituent elements to obtain a systematic behavior of the electric field gradient or magnetic fields within different chemical environments and observe phenomena from an atomic point of view. The hyperfine interactions technique involving the measurement of Perturbed gamma-gamma Angular Correlation (PAC) is being used to investigate a series of intermetallic compounds and metal oxides which present interesting properties like superconductivity, magnetic order, phase transitions, etc.

The PAC techniques uses radioactive nuclei, implanted in the solids, which can probe magnetic hyperfine field (mhf) and electric field gradient (efg) in determined sites of crystalline structure of the material and provide informations about the crystal structure and the origin of the magnetic field.

Due to the proximity of a nuclear research reactor, our laboratory can use a variety of special radioactive probe nuclei such as 140La, 111Ag, 111mCd besides the usual ones like 111In and 181Hf. A second 4-BaF2-detector spectrometer was setup in the laboratory, which incorporated improvements in the electronics and a 6-detectors spectrometer has been designed in order to maximize the detection efficiency. A new methodology for the implantation of the nuclear probe in the sample was developed. This methodology uses the 6Li ion beam from the Pelletron accelerator in IFUSP to implant 111In into the sample through 108Pd(6Li,3n)111In nuclear reaction. The compounds which are being investigate are: oxide compounds: The PAC technique has been used to study the hyperfine interactions in the magnetic and paramagnetic regions of the distorted perovskites LaTO3 where T=Cr, Fe, Co, Mn, using dilute 111In→111Cd and 181Hf→181Ta nuclear probes which were introduced into the samples through a chemical process and 140La→140Ce by irradiating the sample with neutrons.

Temperature dependence of the electric quadrupole interaction parameters as well as the magnetic hyperfine field was obtained for each compound. Rare-earth based compounds series of intermetallic compounds based on rare earth elements show different magnetic behaviors and exhibit very interesting physical phenomena like Fermi liquid behavior, Kondo effect, etc. These properties are not well understood yet, and nuclear techniques are very suitable to investigate the microscopic origin of such phenomena. In our laboratory, we have studied heavy fermion compounds CeIn3, CeMn2Ge2 and CeMn2Si2 using PAC technique using 140Ce and 111Cd probe nuclei.

Other families of intermetallic compounds such as RAg , RNiIn and RPdIn where R is a rare earth element are also being investigated. Ab-initio calculations: The hyperfine interaction parameters can be better understood if the electronic structure of the material is known. A very precise ab-inito method of electronic structure calculations based on the density functional theory using a local density approximation is being used to help in the interpretation of Hyperfine interaction parameters through the WIEN97 code. The first-principles full potential linear augmented plane-wave (FP-LAPW) calculations of the electronic structure and hyperfine fields have been performed for the intermetallic compounds CeIn3 and CeMn2Ge2 CeMn2Si2.

A study of the changes induced by the presence of Zn or Ni impurity at Cu site in CuAlO2 delafossite was also carried out by using FP-LAPW calculations. Ab-initio calculations for the series of compounds like RAg have been initiated.