Materials Characterization with Radioactive Nuclear Techniques

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A **laboratory infrastructure** on materials characterization is maintained and developed at ISOLDE-CERN by the Advanced Materials Research Group of ITN and CFNUL. ISOLDE is a European Large Scale Facility where more than 750 isotopes and 80 elements are produced and delivered as ion beams of high isotopic purity, which is unique in the world. In this context nuclear techniques such as Emission Channeling (EC) and Perturbed Angular Correlations (PAC) provide complementary atomic scale information to the material analysis capabilities available at ion beam laboratories. The ITN-CFNUL infrastructure and related projects are refereed and reevaluated each year within the scope of FCT-supported CERN projects. The scientific work in 2009 was centered in the following research subjects approved by the ISOLDE Scientific Committee:

a) IS453 (U.Wahl) "Emission Channeling Lattice Location Experiments with Short-Lived Isotopes". The lattice sites of dopants and impurities in scientifically and technologically relevant semi-conductors (e.g., Si, Ge, ZnO, GaN and GaAs) are studied by means of the EC technique. Important elements, which have only suitable short-lived isotopes can now be studied, as in the particular case of the ^{27}Mg (9.5 min) isotope, which was for the first time successfully tested in 2009.

b) IS487 (V. Amaral) "Study of Local Correlations of Magnetic and Multiferroic Compounds". PAC is used to study a large variety os multiferroic $RMnO_3$ (R = rare-earth) manganites and cromites $ACrO_2$ (A = Ag, Cu) as a function of the elements R, A, and of temperature. By combining PAC data with first principle simulations of charge density distributions on these materials, local phenomena that correlate the coexistence of ferroelectricity, ferromagnetism and ferroelasticity are studied. 2009 was a year of innovation on the materials being studied, together with the development of new analyzing tools. A new program was developed from scratch that will allow fitting PAC spectra as shaped by dynamic hyperfine interactions, which reveal the existence of transient fields on the materials to study.

c) On a different subject, first experiments regarding proposal IS481 (K. Lorenz) "The role of In in III-nitride ternary semiconductors", have combined γ-γ with e^--γ PAC using the ^{111m}Cd/^{111}Cd and the ^{117}Cd/^{117}In isotopes. The aim is to study the intrinsic nature of In defects in GaN and AlN, with isotopes, which are unambiguously free of "after effects".

In what R&D projects are concerned, first electron detection tests were successfully done with a highly pixelated 512×512 28×28 mm^2 Si detector (TimePix) using both low and high-energy conversion electron and beta sources. In parallel, a new high-resolution goniometer from Panmure, dedicated to on-line experiments with short-lived isotopes, was delivered in 2009. This allowed the planning and design of the special standing and support system as well as of the annealing station to be commissioned at the on-line emission chamber in 2010.

Of interdisciplinary nature, these activities integrate and initiate students from different backgrounds and universities, in applied nuclear physics. With shared work between the different environments of ITN, CFNUL and ISOLDE – CERN, there participate students and senior researchers from the universities of Lisbon, Aveiro, Porto, Braga, ISEL as well as from Leuven in Belgium. During 2009 two Ph.D. and two M.Sc. students defended their thesis; four other Ph.D. and three M.Sc. students performed their work using this infrastructure within the scientific proposals and R&D projects.

Research Team

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IS453 experiment: Emission channelling lattice location studies

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Objectives

The aim of this work is to study the lattice location of dopants and impurities in technologically relevant semiconductors and oxides by means of electron emission channelling (EC) from radioactive isotopes. With this technique information is available for very low dopant concentrations and independent from the host lattice elemental composition. The experiments are carried out using the ITN/CFNUL infrastructure installed at CERN's ISOLDE facility.

Results

1. Lattice location of transition metals in Ge

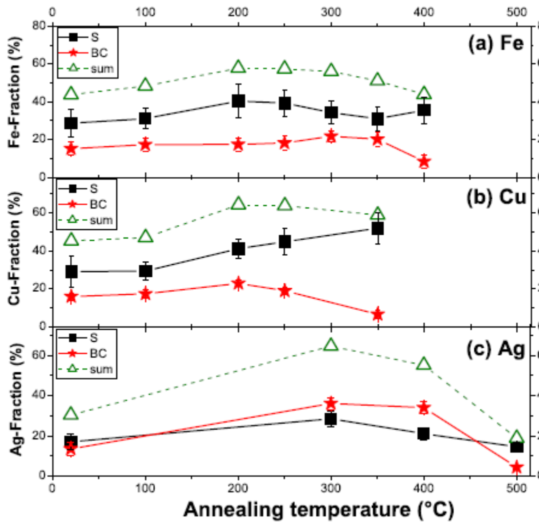

Fig.1 Fractions of implanted ^{59}Fe (45 d), ^{67}Cu (62 h) and ^{111}Ag (7.5 d) probes on S and BC sites in Ge, together with the total fraction (sum = S + BC), as a function of annealing temperature.

We have determined the lattice location of transition metals (TMs) following room temperature implantation into undoped Ge with an energy of 60 keV to fluences around 5×10^{12}–1×10^{13} cm^{-2}. It was found that Fe, Cu, and Ag do not exclusively occupy substitutional sites but bond-centered (BC) sites as well. In order to understand these experimental results, the heat of formation and most stable structural configuration of the following three Cu, Fe and Ag-related complexes in Ge was calculated using ab initio density functional theory: TM on the substitutional S site, TM on the tetrahedral interstitial (T) site, and TM paired with a Ge vacancy (S+V). Corroborated by theory, the BC fraction is attributed to impurity-vacancy complexes in the so-called "split-vacancy" configuration. It was concluded that mobile vacancies, created in our case during the ion implantation process, will be trapped by substitutional impurities, resulting in the spontaneous occupation of the BC site. This result contributes significantly to the understanding of the properties of transition metals in germanium, in particular their interaction with vacancies, which are known to be introduced in some processing steps of Ge technology.

2. Emission channelling with short-lived isotopes

Using our emission channelling on-line setup, which is now mounted permanently at the ISOLDE GHM beamline, we performed a number of lattice location experiments with short-lived radioactive isotopes. During the 2009 Mn beam time we determined the lattice location of ^{56}Mn (1.5 h) implanted into Si as a function of annealing up to 800 °C. It was found that substitutional Mn is dominant, while interstitial Mn cannot be quenched in large amounts. Surprisingly the behaviour of Mn in Si is more similar to Cu than it is to Fe (which we have studied previously). We have recently performed also the first direct lattice location experiments of the magnesium acceptor in nitride semiconductors. For that purpose short-lived ^{27}Mg (9.5 min) probes, which were extracted from a proton-irradiated SiC target by thermal outdiffusion and ionized in a laser ionization source, were implanted with 50 keV into single-crystalline GaN and AlN thin films. The β^- emission channelling patterns showed that the large majority of implanted Mg is incorporated in to Ga or Al sites. Preliminary analysis of the GaN data by .means of fitting the experimental patterns to the results of simulations for ^{27}Mg in different lattice sites gave no indication for large fractions of Mg in interstitial sites.

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