Abstract

The magnetism of single impurity atom in different hosts has been a subject of interest for years. In spite of great deal of efforts, our current understanding regarding magnetism is still incomplete. Although the underlying importance of the Coulomb interactions recognized, there is no universal mechanism for understanding the phenomenon. The point of view taken in this approach is to attempt to understand the magnetic properties of a single impurity in some metals and compounds of immense current interest.

Magnetism generally requires partially filled d or f shells, which by some kind of exchange interaction give rise to magnetic moment formation. Microscopic studies on the occurrence and stability of magnetic moments of partially filled d/f ions in metallic systems and their cooperative interaction leading to different types of magnetic order have an important aspect in the study of magnetism. Generally, some 3d and 4f atoms possess magnetic moments both in elemental form and in alloys due to their partially filled and localized 3d or 4f electronic shells. The survival of magnetic moment on a d or f ion when dissolved in a metallic matrix depends on the competition between the on-site Coulomb interaction U and the virtual line width Δ.

Conventional studies of local magnetism are based on simple metals or metallic alloys. From the vast accumulation from literature, we have chosen four kinds of materials: nano materials, superconducting material and some pure elements from the periodic table, which would provide a new dimension to the local magnetism study.

In this thesis work, we have studied the local magnetic behaviour of isolated impurities in (i) nanocrystalline Nb, (ii) $CaFe_2As_2$, the parent compound of recently discovered ferro pnictides, (iii) highly oriented pyrolytic graphite (HOPG), and (iv) Gd metal. The size induced moment formation has been found to be a novel phenomenon. Reduction in the particle size causes an increase in unit cell volume, thereby reducing the hybridization strength, and ultimately the evolution of a local moment. From the hyperfine interaction studies in $CaFe_2As_2$, we establish that a local moment exists in the paramagnetic state of the material, and both commensurate and incommensurate magnetic ordering is possible below the magnetic phase transition. Through the non magnetic impurity probe in HOPG, we confirm that the bulk of the graphite remains non magnetic, while the near surface region may show an enhanced paramagnetism due to unsaturated bonds. We have in addition provided a general behaviour of transition metal impurities in Gd.

We have used gamma ray time differential perturbed angular distribution (TDPAD) technique, which has been found to be well established method for local investigations and has been used for decades. The experimental results are well supported by *ab initio* calculations based on density functional theory (DFT).

Keywords: Coulomb interaction, local magnetism, virtual line width, commensurate and incommensurate magnetic ordering