Developing a Combined ^{105}Pd NMR and XRD/Neutron Diffraction Approach to Enable the Study of Pd Metal Nanoparticle Systems Used in Industrial Catalytic Processes

An ability to clearly relate local (short range) structure to the function of any material is a critical feature for any catalytic system. The accessible Pd oxidation states, its flexibility of handling and relatively lower cost in comparison to other precious metals makes Pd a viable option in many catalytically driven industrial and technological processes. The most prominent catalytic applications of Pd metal involve its utilisation in the hydrogenation reactions of fatty acids, the cracking of petrochemical systems, and the NO_x/SO_x reduction and the abatement of other Greenhouse gas emissions in automotive car exhaust catalytic converters. This project represents development of the ^{105}Pd solid state NMR technique, and its implementation towards the study of Pd metal nanoparticle systems that are key to these catalytically driven industrial and environmental processes. The very large ^{105}Pd quadrupole parameters (C_Q, η_Q) and the Knight shift (K_{iso}) are very sensitive probes of the small structural distortions within the Pd nanoparticle structure; these structural features will be correlated with the electronic structure and overall catalytic activity of the system. Many surprising observations are able to be elucidated from the ^{105}Pd NMR technique which appear to conflict with the longer range averaged information derived from diffraction techniques.

In this project, the combined use of short range (^{105}Pd solid state NMR) and longer range (XRD/neutron diffraction) information, in conjunction with other materials characterisation techniques (vibrational spectroscopies, etc.) will be used to study Pd nanoparticle systems such as Pd sponge, Pd black and organically capped/stabilised Pd nanoparticles to assess the real bulk and surface-like structural characteristics that influence catalytic activity. To complement these project activities, the PhD student will spend a significant proportion of time interacting with the industrial sponsor (Johnson Matthey) to understand the production processes and measurement of catalytic activity throughout the course of the PhD candidature. Furthermore, there will be an option available for this student to enter the Warwick/NTU (Singapore) Joint PhD Programme where a 12-18 month portion of the 4 year studentship will be spent in a student exchange with NTU School of Materials Science & Engineering. This option will lead to the award of a joint PhD degree between these participating Institutions.