Palladium-defect complexes in diamond and silicon carbide

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Abstract Time Differential Perturbed Angular Correlations (TDPAC) studies, supported by Density Functional Theory (DFT) modelling, have shown that palladium atoms in silicon and germanium pair with vacancies. Building on these results, here we present DFT predictions and some tentative TDPAC results on palladium-defect complexes and site locations of palladium impurities in diamond and silicon carbide. For both diamond and silicon carbide, the DFT calculations predict that a split-vacancy V-PdBI-V complex is favoured, with the palladium atom on a bond-centred interstitial site having a nearest-neighbour semi-vacancy on either side. Consistent with experimental results, this configuration is also assigned to palladium complexes in silicon and germanium. For silicon carbide, the DFT modelling predicts furthermore that a palladium atom in replacing a carbon atom moves to a bond-centred interstitial site and pairs with a silicon vacancy to form a complex that is more stable than that of a palladium atom which replaces a silicon atom and then moves to a bond-centred interstitial site pairings with a carbon vacancy. These two competing alternatives differ by 8.94 eV. The favourable pairing with a silicon vacancy is also supported independently by TRIM Monte Carlo calculations, which predict that more silicon vacancies than carbon vacancies are created during heavy ion implantation.

Keywords Semiconductor defects · Diamond · Silicon carbide · Perturbed angular correlation · Density functional theory

Mathematics Subject Classifications 71.15.-m · 61.72.-y · 71.55.-i · 76.80.+y
1 Introduction

The demand for smaller, lighter and better-performing semiconductor devices has resulted in miniaturization in silicon-based device technology [1, 2]. While silicon-based CMOS technology is presently the manufacturing standard, the fundamental properties of the silicon semiconductor are likely to limit any further miniaturization [3]. Wide band gap semiconductors could be alternative materials to maintain the production of smaller and improved electronic devices [4]. They have the potentials to offer superior materials properties for electronic devices, such as larger thermal conductivity, dielectric strength, and electron saturation velocity in comparison to silicon. Although there are still several technical and fundamental limitations that prevent their competitiveness with the well established silicon-based technology, they still find applications in some important devices, such as high-power, high-temperature, opto-electronic, high-frequency [5, 6], and spintronic [7, 8] devices. There is currently a high demand for devices to operate under extreme conditions. Diamond and silicon carbide (SiC) are two wide band gap semiconductors that are leading candidates for such applications [9, 10].

Diamond is a wide band gap semiconductor with high saturated carrier velocities, high electric field breakdown strength, low dielectric constant and high thermal conductivity. It is the superior material for high power and high temperature electronic applications [11, 12]. These applications will require relatively large surface area substrates, which are likely to be provided by synthetically grown diamonds. SiC has strong potential applications in high-power and high temperature devices as well. It is well known for its polypeptide structures that vary from cubic zinc blende (3C) to wurtzite (2H). Historically, transition metals (TMs) such as titanium, vanadium, and chromium are common impurities in crystalline SiC grown by the Lely technique and have been thoroughly investigated by various experimental methods [13–15].

Likewise, in recent times, TM induced crystallization has been explored for the processing of complementary metal-oxide-semiconductor (CMOS) technology based on germanium (Ge) and Silicon (Si) [16, 17]. Palladium (Pd) has been shown to induce crystallization at a lower temperature than most metals, and therefore has been of a particular interest [17, 18]. In particular, TDPAC and DFT studies have shown that Pd atoms tend to pair in silicon and germanium with nearest neighbour vacancies (V) [19–24]. In similar manner, in the present work TDPAC and DFT studies have been performed on diamond and 3C-SiC.

2 Experimental details

The diamond sample was a high-purity chemical vapour deposition (CVD) grown polycrystalline sample produced by high power microwave deposition on a silicon substrate which was removed after growth. The nitrogen concentration in the diamond was <5ppm. The average crystallite size in the samples was ≈ 100 μm, which is much larger than the estimated maximum implantation range (<2 μm) of the 100Pd ions. The SiC sample was a zinc blende (3C) type single crystal wafer.

The 14UD Pelletron accelerator of the Australian National University was used to synthesize the 100Pd(→100Rh) probe using the 92Zr (12C, 4n)100Pd fusion evaporation reaction. A 70 MeV 12C5+ beam was incident on a 2.5 μm thick zirconium target over 20 hours at a beam current of about 1 μA [25]. Along with other reaction products, 100Pd(→100Rh) probes were directly recoil-implanted into the samples. The probe ions had energies of up to 8 MeV. The samples were placed several millimetres outside the beam path beyond...