Identification of the nature and orientation of palladium-defect pairs in germanium with Perturbed Angular Correlation Spectroscopy of ^{100}Pd/Rh

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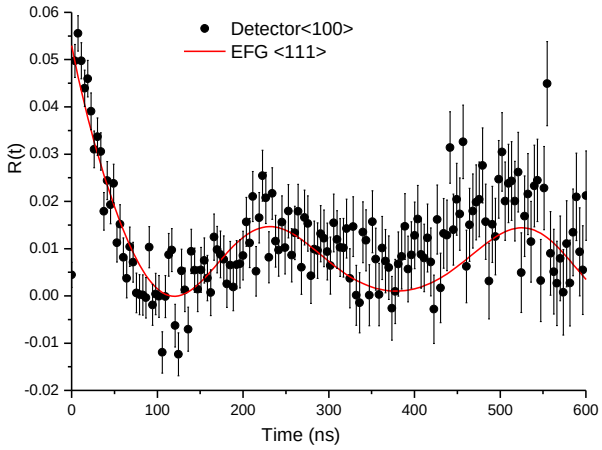
Metal-induced crystallisation of germanium is a promising alternative to silicon in complementary-metal-oxide-semiconductor technology. Palladium is well suited to induce such crystallisation at low temperature. It is, however, not clear how any residual Pd-atoms are integrated in the Ge-lattice, where they may affect electronic properties of the material.

Using the ^{100}Pd/Rh probe Time Differential Perturbed Angular Correlation (TDPAC) Spectroscopy is being pursued to identify the nature of palladium-defect pairs. The probe is synthesized via the fusion evaporation reaction ^{92}Zr(^{12}C,4n)^{100}Pd with the 14UD Pelletron at the Australian National University and recoil-implants into germanium samples.



The data show that a substitutional palladium atom in germanium tends to pair in with a defect following annealing of implantation damage. The quadrupole interaction frequency is 8.3(2) Mrad/s [1]. TDPAC orientation measurements of the ratio function *R(t)*, as shown on the left, are consistent with the defect-pair being oriented in the <111> direction of the germanium lattice.

Further measurements, using the in-beam mass-separator *Solitaire* to reduce implantation damage, are planned. In addition, *Density Functional Theorem* calculations using the codes *QuantumESPRESSO* und *Wien2K* are being pursued to understand the nature of the defect that pairs with palladium, which is expected to be a vacancy [2].

[1] H. Timmers, W. Kemp, A. P. Byrne, M. C. Ridgway, R. Vianden, P. Kessler, M. Steffens, *Hyperfine Interactions* **197**, 159 (2010).
[2] R. Dogra, A. P. Byrne and M. C. Ridgway, *Journal of Electronic Materials* **38,** 623 (2009).

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