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Lattice location and thermal stability of the implanted transition metals Fe, Co and Ni in silicon of different doping types

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Although vacancy-type defects are known to getter transition metals (TMs) in silicon, detailed information on their interaction, e.g. the lattice sites occupied by the TM trapped in the defects, is still poor. Emission Channeling (EC) is a technique that allows us to obtain the preferred sites of the TMs inside these vacancy-type complexes by implanting single crystals with radioactive probe atoms that decay by the emission of beta particles. On their way out of the crystal, beta particles experience channeling effects along crystallographic directions, depending on the lattice site occupied by the probe atom. In this work, we have studied the lattice location of the transition metals 59Fe (t1/2 = 45 d), 61Co (t1/2 = 1.6 h) and 65Ni (t1/2 = 2.5 h) in Si single crystals of various doping types (i, n+, p+) by means of EC at the ISOLDE facility/CERN.

By comparing our two-dimensional experimental patterns with simulations we obtained direct evidence of Fe [1,2], Co and Ni occupying at least three different lattice sites: ideal substitutional (S), displaced bond-center (near-BC) and displaced tetrahedral interstitial sites (near-T). We show that the stability of some sites depends on the doping of the material, e.g. near-BC sites are more stable in n+-type than in p+-type Si. Although we observed the same lattice sites for the three transition metals, some differences can also be found. In particular, while Ni is trapped in near-T sites only after high temperature anneals for all the doping types of silicon, Fe and Co seem to prefer near-T sites in p+-type Si even at room temperature. This can be partially explained by the pairing of Co and Fe with the dopant B in near-T sites, while Ni seems not to respond to the negatively charged dopant. Also, while Fe and Co show considerable stability against annealing even at 900℃, Ni starts to show partial out-diffusion from the samples already in the 600-700℃ range, indicating that vacancy-type defects are less stable gettering centers for Ni than for Fe and Co.

[1] U. Wahl et. al., PRB 72 014115 (2005)
[2] D. J. Silva et. al., JAP 114 103503 (2013)

Primary author: DA SILVA, Daniel (IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia da Faculdade de Ciências da Universidade do Porto, Portugal)

Co-authors: Mr COSTA, Angelo (Instituto Superior Técnico/Instituto Tecnológico e Nuclear, Universidade de Lisboa, Portugal); Mr BOSNE, Eric David (Universidade de Aveiro, Portugal); MARTINS CORREIA, Joao (Instituto Superior Técnico/Instituto Tecnológico e Nuclear, Universidade de Lisboa, Portugal); ESTEVES DE ARAUJO, Joao Pedro (IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia da Faculdade de Ciências da Universidade do Porto, Portugal); PINTO DE ALMEIDA AMORIM, Ligia (Instituut voor Kern-en Stralingsfysica, Leuven, Belgium); DA COSTA PEREIRA, Lino Miguel (Instituut voor Kern-en Stralingsfysica, Leuven, Belgium); CASTRO RIBEIRO DA SILVA, Manuel (Centro de Física Nuclear da Universidade de Lisboa, Portugal); Dr WAHL, Ulrich (Instituto Superior Técnico/Instituto Tecnológico e Nuclear, Universidade de Lisboa, Portugal); AUGUSTYNS, Valerie (Instituut voor Kern-en Stralingsfysica, Leuven, Belgium)

Presenter: DA SILVA, Daniel (IFIMUP and IN-Institute of Nanoscience and Nanotechnology, Departamento de Física e Astronomia da Faculdade de Ciências da Universidade do Porto, Portugal)

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