



Contribution ID: 113

Type: POSTER

Chemical states of ^{57}Fe in rock salt type crystals arising from ^{57}Mn

Chemical states of ^{57}Fe in NaF, NaCl, MgO

Please specify whether you would prefer an oral or poster contribution.

poster

Summary

A study of ^{57}Fe in-beam Mössbauer spectroscopy using ^{57}Mn was applied to the samples having rock-salt type crystal structure, NaF, NaCl and MgO.

The ^{57}Mn beam was produced as a nuclear projectile fragment of the ^{58}Fe beam, and implanted into a sample after passing through Pb/Al/acrylic plate degrader. A sample with 5mm in thickness was used. The ^{57}Fe Mössbauer spectrum of ^{57}Mn implanted into NaF measured at room temperature was relatively simple, which was fitted into the combination of a singlet ($IS = -1.28$ mm/s) and a doublet ($IS = -1.17$ mm/s, $QS = 1.52$ mm/s). The singlet peak is assigned to high-spin Fe^{2+} surrounded by six F^- ions, which substitute Na^+ in NaF crystal. Whereas the assignment of the doublet is difficult; it might be an Fe atom with vacancy of F^- ions in neighbor, or an Fe atom in interstitial position of NaF lattice. NaCl showed a similar spectrum consisting of a singlet ($IS = -1.12$ mm/s) and a doublet ($IS = -1.11$ mm/s, $QS = 1.41$ mm/s). The singlet corresponded to the substitutional site and the doublet to a defect or interstitial site. The spectrum of MgO was analyzed as the sum of a singlet and doublets. Density functional calculations using ADF program set applying cluster model were performed to estimate the electronic structure of the Fe atom in NaF lattice in various environment in order to make an assignment of the doublet peaks.

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Track Classification: Biology, Chemistry, Medicine