

Local Environment and Electronic Structure in K_2NiF_4 -type $La_2Li_{0.50}Cu_{0.50}O_4$ Doped by ^{57}Fe

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The ^{57}Fe Mössbauer spectrum of the oxide $La_2Li_{0.50}Cu_{0.50}O_4$ doped with ^{57}Fe (1 at.-%) underlines at 300 K the presence of three different components: two corresponding to the substitution of ^{57}Fe probe atoms for respectively “ Cu^{3+} ” [Fe(1)] and Li^+ [Fe(3)] and the third [Fe(2)] attributed to ^{57}Fe associated with oxygen vacancies. A decrease of the temperature down to 77 K does not lead to essential changes of the Mössbauer parameters corresponding to the Fe(1) and Fe(2) sub-spectra. On the contrary, a drastic change occurs in the Fe(3) sub-spectrum which has been interpreted by a displacement of the charge-transfer equilibrium $Fe^{4+}(3) + O^{2-} \rightarrow Fe^{3+}(3) + O(\underline{L})$ at the Li^+ sites.

Key words: Solid State, Electronic Structure, ^{57}Fe Mössbauer Spectroscopy,
 K_2NiF_4 -type Compound