

НИИ ФИЗИКИ ЮЖНОГО ФЕДЕРАЛЬНОГО УНИВЕРСИТЕТА

**МЁССБАУЭРОВСКАЯ СПЕКТРОСКОПИЯ И ЕЕ
ПРИМЕНЕНИЯ**

**Сборник материалов
XV Международной конференции**



Сочи, 10— 16 сентября 2018 г.

Ростов-на-Дону
2018

УДК 548.9 + 53.043 + 543.429.3
ББК

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M53 Мёссбауэровская спектроскопия и ее применения: сборник материалов XV Международной конференции (Сочи, 10–16 сентября 2018 г.); Южный федеральный университет. – Ростов-на-Дону ; Таганрог : Издательство Южного федерального университета, 2018. – 188 с илл.
ISBN 978-5-9275-2831-8

Сборник включает в себя программу и тезисы докладов участников XV Международной конференции «Мёссбауэровская спектроскопия и ее применения», проводившейся в г. Сочи 10 – 16 сентября 2018 г.

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ББК

ISBN 978-5-9275-2831-8

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Mössbauer study of iron-based superconductor $\text{Fe}_{1.09}\text{Se}_{0.5}\text{Te}_{0.5}$

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Since discovery of superconductivity in iron-based compounds [1], the iron selenide is in the focus of world-wide investigations of iron-based superconductors. Numerous papers reported that superconducting transition critical temperature of Te-doped FeSe increases [2, 3]. At room temperature, FeSe and FeTe compounds have quite similar layered crystal structure that simplifies Te-doping of FeSe compound [3]. Nevertheless, it is well known that $\text{Fe}_{1+y}(\text{Se}_{1-x}\text{Te}_x)$ systems always contains excess iron atoms which affect the electronic and magnetic properties. The recent neutron diffraction studies of a number of $\text{Fe}(1+y)\text{Te}$ samples have shown that presence of the excess iron (y) complicates the magnetic ordering in these systems [4]. It was reported for $\text{Fe}_{1.05}\text{Te}$ system that the excess iron atoms lead to appearance of four nonequivalent centers of iron atoms with different hyperfine parameters [3].

We present Mössbauer studies of the influence of excess iron atoms on the properties of ironbased superconductor $\text{Fe}_{1.09}\text{Se}_{0.5}\text{Te}_{0.5}$. Mössbauer spectra were collected in a temperature range from liquid helium up to room temperature. The temperature dependences of hyperfine parameters was investigated. The Mössbauer spectra have shown a complex shape and could be treated with a model based on first principle density functional theory calculation results similar to that in Ref. [3]. The reported study was funded by RFBR according to the research project No 18-32-00342.

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