

# Mössbauer spectroscopy evidence of intrinsic non-stoichiometry in iron telluride single crystals

Kiiamov A., Lysogorskiy Y., Vagizov F., Tagirov L., Tayurskii D., Croitori D., Tsurkan V., Loidl A.  
*Kazan Federal University, 420008, Kremlevskaya 18, Kazan, Russia*

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## Abstract

© 2016 by WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim The FeTe parent compound for iron-superconductor chalcogenides was studied applying Mössbauer spectroscopy accompanied by ab initio calculations of electric field gradients at the iron nuclei. Room-temperature (RT) Mössbauer spectra of single crystals have shown asymmetric doublet structure commonly ascribed to contributions of over-stoichiometric iron or impurity phases. Low-temperature Mössbauer spectra of the magnetically ordered compound could be well described by four hyperfine-split sextets, although no other foreign phases different from Fe<sub>1.05</sub>Te were detected by XRD and microanalysis within the sensitivity limits of the equipment. Density functional ab initio calculations have shown that over-stoichiometric iron atoms significantly affect electron charge and spin density up to the second coordination sphere of the iron sublattice, and, as a result, four non-equivalent groups of iron atoms are formed by their local environment. The resulting four-group model consistently describes the angular dependence of the single crystals Mössbauer spectra as well as intensity asymmetry of the doublet absorption lines in powdered samples at RT. We suppose that our approach could be extended to the entire class of Fe<sub>1+y</sub>Se<sub>1-x</sub>Te<sub>x</sub> compounds, which contain excess iron atoms. (Figure presented.)

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## Keywords

ab initio, iron chalcogenides, mössbauer spectroscopy

## References

- [1] Y. Kamihara, T. Watanabe, M. Hirano, and H. Hosono, *J. Am. Chem. Soc.* 130(11), 3296–3297 (2008).
- [2] J. Paglione and R. L. Greene, *Nat. Phys.* 6, 645–658 (2010).
- [3] G. R. Stewart, *Rev. Mod. Phys.* 83(4), 1589 (2011).
- [4] X. Chen, P. Dai, D. Feng et al., *Nat. Sci. Rev.* 1, 371–395 (2014).
- [5] F. C. Hsu, J. Y. Luo, K. W. Yeh et al., *Proc. Nat. Acad. Sci.* 105(38), 14262–14264 (2008).
- [6] Y. Mizuguchi, F. Tomioka, S. Tsuda et al., *Appl. Phys. Lett.* 93(15) (2008).
- [7] S. Medvedev, T. McQueen, I. Troyan et al., *Nat. Mater.* 8(8), 630–633 (2009).
- [8] M. Fang, H. Pham, B. Qian et al., *Phys. Rev. B* 78(22), 224503 (2008).
- [9] A. Martinelli, A. Palenzona, M. Tropeano et al., *Phys. Rev. B* 81(9), 094115 (2010).
- [10] F. Gronvold, H. Haraldsen, and J. Vihovde, *Acta Chemica Scand.* 8(10), 1927–1942 (1954).
- [11] D. Finlayson, D. Greig, J. Llewellyn, and T. Smith, *Proc. Phys. Soc. Sec. B* 69(8), 860 (1956).
- [12] L. Zhang, D. J. Singh, and M. H. Du, *Phys. Rev. B* 79(1), 012506 (2009).

- [13] E. E. Rodriguez, C. Stock, P. Zajdel et al., *Phys. Rev. B* 84(6), 064403 (2011).
- [14] M. Enayat, Z. Sun, U. R. Singh et al., *Science* 345(6197), 653-656 (2014).
- [15] R. Viennois, E. Giannini, D. VanDer Marel, and R. Černý, *J. Solid State Chem.* 183(4), 769-775 (2010).
- [16] S. Cao, S. Shen, L. Chen et al., *J. Appl. Phys.* 110(3), 033914 (2011).
- [17] G. Chen, Z. Chen, J. Dong et al., *Phys. Rev. B* 79(14), 140509 (2009).
- [18] M. Z. Cieplak and V. Bezusyy, *Phil. Mag.* 95(5-6), 480-492 (2015).
- [19] J. Li, G. Huang, and X. Zhu, *Physica C: Supercond.* 492, 152-157 (2013).
- [20] M. J. Han, Q. Yin, W. E. Pickett, and S. Y. Savrasov, *Phys. Rev. Lett.* 102(10), 107003 (2009).
- [21] H. Shi, Z. B. Huang, S. T. John, and H. Q. Lin, *J. Appl. Phys.* 110(4), 043917 (2011).
- [22] M. Monni, F. Bernardini, G. Profeta, and S. Massidda, *Phys. Rev. B* 87(9), 094516 (2013).
- [23] F. Ma, W. Ji, J. Hu et al., *Phys. Rev. Lett.* 102(17), 177003 (2009).
- [24] T. Miyake, K. Nakamura, R. Arita, and M. Imada, *J Phys. Soc. Jap.* 79(4), 044705 (2010).
- [25] T. McQueen, Q. Huang, V. Ksenofontov et al., *Phys. Rev. B* 79(1), 014522 (2009).
- [26] Y. Mizuguchi, T. Furubayashi, K. Deguchi et al., *Physica C: Supercond.* 470, S338-S339 (2010).
- [27] R. Gómez, V. Marquina, J. Pérez-Mazariego et al., *J. Supercond. Nov. Magn.* 23(4), 551-557 (2010).
- [28] K. Reddy and S. Chetty, *Phys. Stat. Solidi (a)* 37(2), 687-694 (1976).
- [29] K. Szymański, W. Olszewski, L. Dobrzyński et al., *Supercond. Sci. Techn.* 24(10), 105010 (2011).
- [30] C. Koz, S. Rößler, A. Tsirlin et al., *Phys. Rev. B* 86(9), 094505 (2012).
- [31] D. Louca, K. Horigane, A. Llobet et al., *Phys. Rev. B* 81(13), 134524 (2010).
- [32] S. Li, C. de La Cruz, Q. Huang et al., *Phys. Rev. B* 79(5), 054503 (2009).
- [33] J. Lindén, J. P. Libäck, M. Karppinen et al., *Solid State Commun.* 151(2), 130-134 (2011).
- [34] S. Margulies and J. Ehrman, *Nucl. Instrum. Meth.* 12, 131-137 (1961).
- [35] V. Goldanskii, E. Makarov, and V. Khrapov, *Phys. Lett.* 3(7), 344-346 (1963).
- [36] P. Gütllich, E. Bill, and A. X. Trautwein, *Mössbauer spectroscopy and transition metal chemistry: fundamentals and applications* (Springer Science & Business Media, 2010), 568 p.
- [37] D. Satuła, K. Szymański, L. Dobrzyński, V. Tran, and R. Troć, *Phys. Rev. B* 78(1), 014411 (2008).
- [38] A. Błachowski and U. Wdowik, *Acta Phys. Pol. A* 119(1), 24-27 (2011).
- [39] A. Błachowski and U. D. Wdowik, *J. Phys. Chem. Solids* 73(2), 317-323 (2012).
- [40] G. Kresse and J. Hafner, *Phys. Rev. B* 47, 558 (1993).
- [41] G. Kresse and J. Hafner, *Phys. Rev. B* 49, 14251-14269 (1994).
- [42] G. Kresse and J. Furthmuller, *Comp. Mater. Sci.* 6, 15-50 (1996).
- [43] G. Kresse and J. Furthmuller, *Phys. Rev. B* 54, 11169-11186 (1996).
- [44] P. E. Blöchl, *Phys. Rev. B* 50(24), 17953 (1994).
- [45] J. P. Perdew, K. Burke, and M. Ernzerhof, *Phys. Rev. Lett.* 77(18), 3865 (1996).
- [46] H. M. Petrilli, P. E. Blöchl, P. Blaha, and K. Schwarz, *Phys. Rev. B* 57(23), 14690 (1998).
- [47] P. Schwerdtfeger, T. Söhnel, M. Pernpointner et al., *J. Chem. Phys.* 115(13), 5913-5924 (2001).
- [48] I. Kantor, L. Dubrovinsky, C. McCammon et al., *Phys. Rev. B* 80(1), 014204 (2009).
- [49] D. Welz, P. Deppe, W. Schaefer, H. Sabrowsky, and M. Rosenberg, *J. Phys. Chem. Solids* 50(3), 297-308 (1989).
- [50] M. Nishi, Y. Ito, and A. Ito, *J. Phys. Soc. of Jpn.* 52(10), 3602-3610 (1983).
- [51] H. P. Nissen and K. Nagorny, *Z. Phys. Chem. Neue Folge* 99(4-6), 209-216 (1976).
- [52] A. Błachowski, K. Ruebenbauer, J. Żukrowski et al., *J. Alloy. Comp.* 494(1), 1-4 (2010).
- [53] S. I. Shylin, V. Ksenofontov, S. A. Medvedev, and C. Felser, *J. Supercond. Nov. Magn.* 29(3), 573-576 (2015).
- [54] J. Greneche and F. Varret, *Journal de Physique Lettres* 43(7), 233-237 (1982).