

Evidence of the Plaquette Structure of Fe_{1+x}Te Iron Telluride: Mössbauer Spectroscopy Study

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Single-crystalline Fe_{1+x}Te iron telluride with off-stoichiometric iron has been synthesized by the Bridgman method. The X-ray diffraction and wave-length-dispersive X-ray electron-probe microanalysis characterization have shown $\text{Fe}_{1.125}\text{Te}$ stoichiometry of the samples. Spin-polarized ab initio calculations of the electric field gradients around interstitial iron atoms for $\text{Fe}_{1.125}\text{Te}$ have shown that in the first and second coordination rings around interstitial iron, the spin and electron densities are strongly perturbed against the stoichiometric ones. Together with the interstitial iron this gives rise to three kinds of iron centers making up a round-corner plaquette. The room-temperature Mössbauer spectra measured at different incidence angles of gamma-radiation are satisfactorily fitted utilizing the hyperfine parameters, calculated within the plaquette model. The low-temperature data are well described with the assumption of an incommensurate collinear spin density wave (SDW) phase, showing consistency with neutron scattering data for the $\text{Fe}_{1.125}\text{Te}$ system.

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1. Introduction

The discovery of superconductivity in iron selenide FeSe with a critical temperature of about $T_c \approx 8\text{ K}$ ^[1] has driven worldwide efforts in searching for chalcogenide compounds with higher T_c . It had been predicted that, within a spin-fluctuation derived picture of superconductivity, FeTe with doping should show a higher superconductivity transition temperature than FeSe.^[2] Contrary to the expectations, superconductivity has not been observed in the stoichiometric iron telluride compound. Moreover, it is well known that iron telluride is always synthesized with iron off-stoichiometry^[3–5] – a feature, which attracts very much attention last time (see recent work^[6] and references therein). In our previous study,^[7] the off-stoichiometric iron telluride $\text{Fe}_{1.05}\text{Te}$ was studied making

use of a combination of Mössbauer spectroscopy experiments and ab initio calculations. An essential output of our study in ref. [7] is a four-center model for the local environment of iron ions in the iron-surplus lattice of Fe_{1+x}Te . Spatially, the constituents of the four-center model are located around an interstitial excess iron ion (see Figure 4 of ref. [7]) and form something like a plaquette (see Figure 5 of ref. [7]). It consists of interstitial excess iron ion (Fe2) and two coordination rings (nearest and next-nearest neighbors) of intralayer iron ions (Fe1/1 and Fe1/2, respectively) around it. Depending on the concentration of the excess iron, these plaquettes could be either separated by a rest of unperturbed Fe1 ions at low concentration of Fe2 ions ($\approx 5\%$ and lower), or adjoin one another, or eventually overlap when the concentration increases further. In the case of large concentration of excess Fe2 ions, their strong magnetism^[8] and the plaquette structure around^[7] could be a reason for suppression of spin fluctuations, which mediate the superconductivity in iron-based superconductors, according to ref. [2]. Moreover, the existence of three distinct regions in the phase diagram of magnetic ordering in dependence on the excess-iron concentration^[6] could be a result of the above-mentioned three regimes of the plaquette arrangement.

In this article we present the results of Mössbauer spectroscopy study of highly Fe2 off-stoichiometric iron telluride $\text{Fe}_{1.125}\text{Te}$ sample and its interpretation based on our ab initio calculations to further justify the four-magnetic-center model and the plaquette iron-ion structures in Fe-rich Fe_{1+x}Te

chalcogenides.^[7] The paper is organized as follows: in the next section we describe the sample preparation, characterization, and Mössbauer spectroscopy measurement procedures. The details of ab initio calculations are given in Section 3. The discussion of the measurement results and their description within the four-magnetic-center model are provided in Section 4. Finally, the Section 5 summarizes findings of the present study.

2. Sample Preparation and Experimental Details

For a sample growth the starting materials in the stoichiometry of $\text{Fe}_{1.15}\text{Te}$ was processed as it is described in ref. [7]. The single-crystalline part of the resulted ingot was used for X-ray diffraction analysis (XRD), elemental composition, and Mössbauer spectroscopy studies. The XRD measurements of the crushed single crystals performed at a conventional powder diffractometer (STADI-P, STOE&CIE) did not reveal any impurities. The Rietveld analysis of the XRD pattern shown in **Figure 1** was performed based on the tetragonal lattice of P4/nmm symmetry. The lattice constants were determined as $a = b = 3.83 \text{ \AA}$, $c = 6.27 \text{ \AA}$. The atomic coordinates are presented in **Table 1**. The refined stoichiometry values of iron were 1.007 (± 0.006) and 0.126 (± 0.002) for Fe1 and Fe2 ions, respectively. Single crystal X-ray diffraction analysis confirmed the crystallographic plane (001) to be the surface cleavage plane of the samples.

The composition of the sample has been measured by wavelength-dispersive X-ray electron-probe microanalysis (WDS EPMA, Cameca SX50). The data were averaged over 10 points with the surface of $70 \times 60 \mu\text{m}^2$ measured on different parts of the single crystalline sample. The obtained resulting composition was $\text{Fe}_{1.124(\pm 0.004)}\text{Te}$.

Mössbauer spectroscopy measurements were carried out in temperatures 4.2 and 295 K (RT), using a conventional constant-

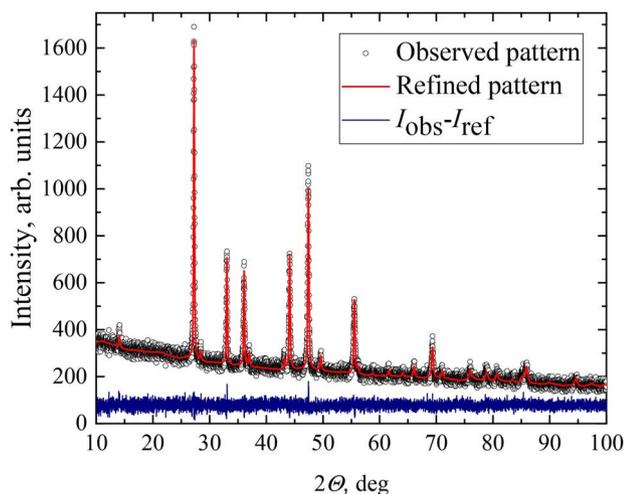


Figure 1. Rietveld refinement of the ground single crystals of Fe_{1+x}Te . Open circles show the observed intensity, red solid line – the calculated pattern, blue line – the difference between the observed and calculated patterns.

acceleration spectrometer (WissEl, Germany) with ^{57}Co of about $40 \mu\text{Ci}$ activity in a rhodium matrix as γ -radiation source. A set of numerous thin flakes, cut from the single-crystal ingot and packed with surface orientation parallel to the cleavage plane (001), was used as a sample (absorber) for the Mössbauer effect measurements. Low-temperature measurements were carried out with a continuous helium-flow cryostat (model CFICEV from ICE Oxford, UK). At RT a metallic-iron foil was used for velocity calibration of the Mössbauer spectrometer. Isomer shifts were referred to α -Fe at RT.

Except a special one, all measurements were carried out at zero angle β between crystallographic c -axis of the sample's crystalline flakes and γ -radiation propagation direction. Besides, one test measurement had been done for the β -angle equal to 54.7° . The non-zero β -angle spectrum was necessary to verify the computational ab initio model proposed below (see Section 3). The Mössbauer spectra were obtained in two velocity ranges: (i) in RT measurements from -2 to $+2 \text{ mm s}^{-1}$ in order to obtain an accurate line shape; and (ii) at low temperatures from -5.3 to $+5.7 \text{ mm s}^{-1}$ to observe all lines of magnetic sextets.

3. Ab Initio Calculation Details

The calculations have been performed by means of density functional theory (DFT) using the Vienna ab initio simulation package (VASP 5.3)^[9–12] integrated into the MedeA software complex. The electron-ion interactions were described by using the projector-augmented wave (PAW) method. The PAW method is a frozen-core one that uses the exact shape of the valence-electron wave functions instead of pseudo-wave functions.^[13] The Perdew–Burke–Ernzerhof (PBE) generalized gradient approximation (GGA) was used for the exchange and correlation corrections.^[14] The Fe ($3d^6 4s^2$) and Te ($5s^2 5p^4$) electrons of the valence shell were treated explicitly, whereas remaining electrons of the cores were taken into account by using pseudopotentials. Plane waves (PW) were included into the basis set up to a cutoff of 500 eV. The k -point mesh was a $9 \times 9 \times 9$ Monkhorst–Pack grid which corresponds to actual k -spacings of $0.091 \times 0.091 \times 0.111$ per \AA . Despite of the fact that Fe-3d electrons are strongly correlated, in ref. [8] it was argued that density functional theory provides a useful starting point for understanding the electronic properties of iron chalcogenide materials, and that its description is not improved by inclusion of additional on-site Coulomb terms which is realized in the GGA + U method. So we restricted ourselves by the GGA approach. Electric-field gradients at the positions of the atomic nuclei were calculated using a method of ref. [15].

Table 1. The atomic coordinates of $\text{Fe}_{1.125}\text{Te}$ sample obtained from XRD data.

Ion	X	Y	Z
Fe1	0.75	0.25	0
Fe2	0.25	0.25	0.714
Te	0.25	0.25	0.286

Despite of the fact that DFT can calculate the ground state only at $T = 0$ K, in order to simulate the system at room temperature, we used the experimental values of the RT lattice parameters and atom positions obtained by XRD. The $2 \times 2 \times 1$ supercell has been used in our consideration. The supercell contains 8 Te atoms and 9 Fe atoms including one excess iron atom (Fe2) and corresponds to composition $\text{Fe}_{1.125}\text{Te}$. Within accuracy limitations of XRD and EDS techniques the $2 \times 2 \times 1$ supercell corresponds to the sample under consideration.

It is known that Fe_{1+x}Te compounds (x up to 0.08) are paramagnetic at room temperature.^[3,16] Indeed, our RT Mössbauer measurements do not indicate any magnetic order. On the other hand, previous ab initio calculations demonstrate that the magnetic moment of excess iron ions in $\text{Fe}_{1.125}\text{Te}$ is calculated to be $2.4 \mu_B$.^[8] So, in order to provide correct consideration of magnetic order in our samples, we have performed spin-polarized calculations. Magnetic moments on all iron ions were initialized with zero value. After calculating the ground state utilizing DFT, the Fe2 iron ions developed into in a magnetic state with $\mu(\text{Fe}2) = 2.3 \mu_B$, while the magnetic moments of the Fe1 iron ions remained almost equal to zero, $\mu(\text{Fe}1) \approx 0$.

4. Results and Discussion

The RT Mössbauer spectra are presented in **Figure 2** and **Figure 3**. It is clearly seen that both of them have asymmetric line shape. It is typical for $\text{Fe}_{1+y}\text{Te}_{1-x}\text{Se}_x$ systems.^[3,16,17] Previously, in $\text{Fe}_{1.05}\text{Te}$, it has been shown that such line shape of Mössbauer spectrum appears as a result of the complex distribution of electric-field gradients (EFG) caused by the presence of excess iron ions Fe2.^[7,18] The EFG were evaluated from the ab initio calculations providing, as it was demonstrated in refs. [15,19,20], semi-quantitative data suitable for the accurate analysis of experimental Mössbauer spectra.^[7]

Our ab initio calculations for the $\text{Fe}_{1.125}\text{Te}$ system have shown the appearance of three groups of different iron ions. These groups have different values of Mössbauer parameters, such as

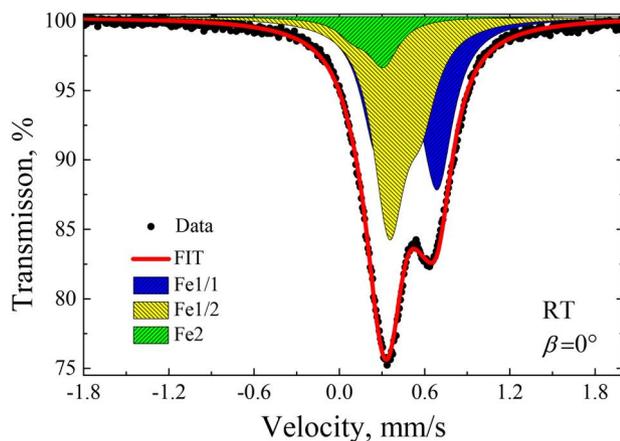


Figure 2. The RT Mössbauer spectrum of single-crystalline $\text{Fe}_{1.125}\text{Te}$ (black solid symbols) and the spectrum fitted within the plaquette structure model (red line).

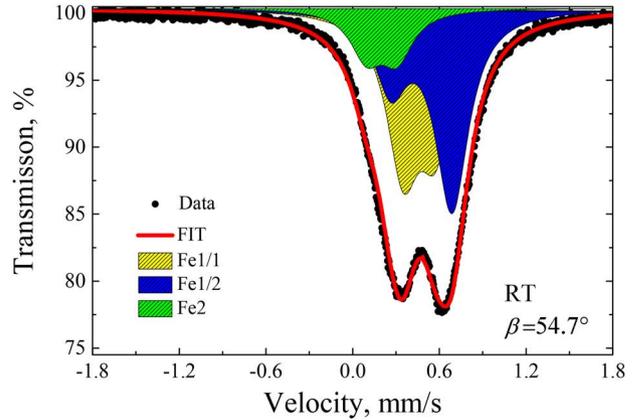


Figure 3. The experimental RT Mössbauer spectrum of the single-crystalline $\text{Fe}_{1.125}\text{Te}$ sample obtained for the β -angle equal to 54.7° (black solid symbols) and the calculated spectrum within the plaquette structure model for $\beta = 54.7^\circ$ (red line).

the asymmetry parameter, the quadrupole splitting and the α -angle between EFG principal axis and the crystallographic c -axis. One of the groups, Fe2 group, contains only Fe2 ions. The other two groups accumulate the first and second coordination rings around the excess iron ions Fe2 – Fe1/1 and Fe1/2 groups, respectively. The relative partial spectrum area of the each group has been calculated as a ratio of the number of iron atoms in the group to the total number of atoms in the supercell. The calculated Mössbauer parameters are collected in **Table 2**.

Isomer shifts (IS) of iron ions were not calculated in the present work. Nevertheless, we suppose that the iron ions of each group should have their particular value of the isomer shift because of different environment. The isomer shift for the iron ions type Fe1 was calculated in ref. [21] for a hypothetical ideal FeTe with zero concentration of excess iron atoms. The value lies in a range between $[0.40 \text{ and } 0.45 \text{ mm s}^{-1}]$ depending on the method of calculation.

Although the ab initio approach allows evaluating of the electric field gradients only semi-quantitatively,^[15,19,20] it catches fundamental information about extent and character of the host lattice perturbation by interstitial Fe2 ions. We utilized the ab initio results for the analysis of the experimental Mössbauer spectra as follows: (i) QS and α for the fitting procedure were taken from ab initio calculations (Table 2) as an initial guess; (ii) the initial value for the isomer shift was taken as $\text{IS} = 0.425 \text{ mm s}^{-1}$ in accordance with ref. [21]; (iii) during the fitting procedure, the QS, α -angle and IS values were varied slightly to better reproduce the experimental spectrum by the proposed model of three groups (natural linewidth 0.097 mm s^{-1} was used

Table 2. The ab initio calculated Mössbauer spectra parameters for $\text{Fe}_{1.125}\text{Te}$.

Group label	Asymmetry parameter η	Quadrupole splitting (mm s^{-1})	α -Angle ($^\circ$)	Relative partial spectrum area
Fe2	0	0.11	0	0.11
Fe1/1	0.46	0.24	49	0.44
Fe1/2	0.11	-0.04	6	0.44

during the fitting procedure). The fitted values of QS, α , and IS are presented in **Table 3**.

As can be seen from comparison of Table 2 and 3, the ab initio calculated values of the α -angle, asymmetry parameter, and relative partial spectral areas agree fairly well with the fitted ones. At the same time, one can notice a significant difference between the calculated and fitted values of QS. Such discrepancy could be a result of several factors: (a) it is known that ab initio simulations by means of density functional theory calculate a ground state of the system only at zero temperature. Nevertheless, the fitting had been done for the spectra measured at room temperature, while a quadrupole splitting is quite temperature-sensitive parameter; (b) it was mentioned above that even for zero-temperature the ab initio calculations provide only semiquantitative accuracy for the quadrupole splitting values.^[15,19,20] We note that, despite of the quantitative discrepancy for the quadrupole splittings, the estimation agrees with the experimental data in terms of sign of the quadrupole splittings, and, moreover, one can see that the calculated quadrupole splittings for the Fe2 and Fe1/1 groups could be adjusted to the experimental values by using a common factor equal to about 2. Nevertheless, the factor fails to scale the low value of the calculated quadrupole splitting of iron ions in the group Fe1/2.

Such disagreement between the QS values for the Fe1/2 ions is a result of location of the atoms at the edge of a cell. The ab initio calculation estimations have been made for the zero-temperature conditions and stationary atoms in the supercell. In this case the Fe1/2 ions are influenced by two equidistantly located Fe2 atoms from each of the neighboring supercells. For Fe1/2 ions at the common edge of two supercells there is mutual compensation of perturbations from each of the Fe2 atoms. On the contrary, the fitted QS values were obtained from the spectra at RT, at which non-stationarity of the atoms in the cells leads to complicated distribution of the charge density and electric-field gradients, and hence, to appearance of significant QS for the edge atoms. Nevertheless, the crystal symmetry dependent EFG parameters, such as α -angle of the EFG principal axes and sign of the quadrupole splitting were estimated quite accurately.

One more feature of the calculation method, which needs to be discussed, is the relative partial spectrum area presented in Table 2. In fact, besides the amount of the iron atoms, these partial spectrum areas depend on the probability of the recoilless gamma-quanta absorption by a nucleus (i.e., Mössbauer effect), which is called Lamb-Mössbauer factor. Generally, the Lamb-Mössbauer factor is a function of the mean-square displacement of atoms depending on the phonon density of states of the atoms. Unlike atoms of the groups Fe1/1 and Fe1/2, located in the crystallographic position $2a$ of iron, the Fe2 group atoms occupy position $2c$, and it is expected that the phonon-mode distributions for atoms of different groups is different that

leads to the disagreement between the calculated and the experimental values of the relative partial spectrum areas. Consideration of double Fe2 centers of excess iron goes beyond the accuracy of our calculations since the probability of the Fe2 pairs is quadratic in the concentration of Fe2 centers (i.e., $(0.125)^2 = 0.0156$ in our case), thus making a total contribution of about one percent to the total spectrum area.

The values of the isomer shift IS for the Fe1/1 and Fe1/2 iron groups are very close to each other (see the last column of Table 3). The IS value for the Fe2 group is somewhat smaller. This fact could be explained by the difference of valence states of Fe1 and Fe2 ions. Reference [8] reported that Fe2 occurs in the Fe^{+} valence state, while Fe1 should have a valence $2+$. Moreover, the IS values for Fe2 ions obtained in refs. [7,16] is also smaller than for Fe1 ions.

The results from Table 3 were used to simulate the Mössbauer spectrum obtained for the β -angle (the angle between c -axis of the crystalline flakes and the γ -radiation propagation) equal to 54.7° . No further fitting procedure has been applied – the model spectrum for $\beta = 54.7^\circ$ was calculated using the parameters of Table 3 obtained for the $\beta = 0^\circ$ geometry. Figure 3 represents a comparison of the experimental spectrum and the simulated one. It could be seen that our model is able to describe the angular dependence of the Mössbauer spectra quite well.

So, we argue that it could be concluded that the $Fe_{1.125}Te$ system contains three different types of iron ions clearly seen in the Mössbauer spectroscopy experiments. The EFG pattern is generally similar to that one in $Fe_{1.05}Te$ system, where four iron ion groups had been seen. Increasing of the concentration of interstitial iron atoms, and therefore, reduction of the room for the plaquette structure, leads to decreasing of the number of groups.

The low-temperature Mössbauer spectrum of the $Fe_{1.05}Te$ system consisted of four magnetic sextets, which were a consequence of four iron ion groups.^[7] For the $Fe_{1.125}Te$ system, a more complex low temperature spectrum is expected because of the presence of spin density waves.^[6] It was reported that the magnetic structure of $Fe_{1.124(5)}Te$ (notations of ref. [6]) is a collinear spin density wave (SDW) phase with incommensurate wave-vector $q = 0.46 \pm 0.01$ (in reciprocal-lattice units (r.l.u.))^[6] along $[H,0,0]$ direction (that corresponds to the x -direction in real space). Such wave-vector value fits the SDW wavelength equal to $(1.085 \pm 0.015) \times a$, where a is the lattice parameter of $Fe_{1.124(5)}Te$ ($a = 3.83 \text{ \AA}$). For such magnetic order, a superstructure with somewhat about 11 lattice periods contains an integer number of SDW wavelengths.

The value of the incommensurate SDW wave vector $q = 0.46 \pm 0.01$ r.l.u. and the presence of three different groups of iron ions in each of the $2 \times 2 \times 1$ supercells allow us to argue that the low-temperature Mössbauer spectrum of $Fe_{1.125}Te$ should

Table 3. The Mössbauer spectra parameters obtained after fitting the experimental data of Figure 2.

Group label	Asymmetry parameter η	Quadrupole splitting ($mm\ s^{-1}$)	α -Angle ($^\circ$)	Relative partial spectrum area	Isomer shift ($mm\ s^{-1}$)
Fe2	0	0.23	0	0.130	0.20
Fe1/1	0.46	0.42	46	0.435	0.48
Fe1/2	0.11	-0.22	8	0.435	0.46

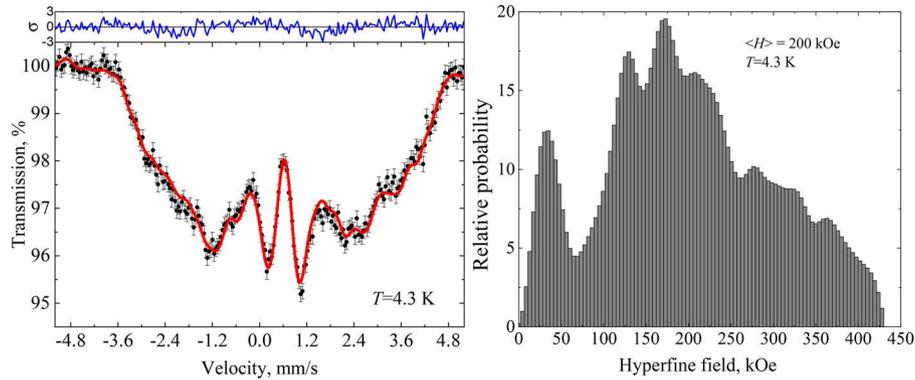


Figure 4. (Left) Mössbauer spectrum of $\text{Fe}_{1.125}\text{Te}$ single crystalline sample obtained at 4.3 K and fitted by a distribution of hyperfine fields (shown in the right panel). The difference between the experimental and simulated spectra is shown by a thin blue line on top. (Right) The distribution of hyperfine fields, see discussion in Section 5.

show a complex superposition of numerous sub-spectra. It is reasonable to describe it by a number of sextets with a broad hyperfine field distribution ranging from zero to a maximum field value. The results of such approximation are presented in **Figure 4** (left) and **Figure 5** (left) for the spectra obtained at temperatures of 4.3 and 35 K with average hyperfine field values $\langle H \rangle = 200 \text{ kOe}$ and $\langle H \rangle = 180 \text{ kOe}$, respectively. Figure 4 (right) and Figure 5 (right) present the corresponding hyperfine field distributions. The orientation of magnetic moments in the sample was taken in account during the fitting procedure. Because each flake of the iron telluride in the absorber had been put in a way that γ -radiation propagation direction was perpendicular to the magnetic moment in SDW, the line intensities ratios I_3/I_1 and I_2/I_1 were set to 1/3 and 4/3, respectively. The model shows pretty good fitting to the experimental data in Figure 4 (left) and Figure 5 (left).

5. Conclusion

Spin-polarized ab initio calculations of the electric field gradients around isolated interstitial iron atom Fe2 have shown that spin and electron densities in the layer of adjacent Fe1 ions are

perturbed against stoichiometric ones up to the third coordination ring around the Fe2 ion.^[7] First (Fe1/1) and second (Fe1/2) coordination rings are significantly affected by this perturbation, and together with interstitial Fe2 form three kinds of iron centers making up something like a corner plaquette (see Figure 5 of ref. [7]). The third coordination ring of Fe1 atoms is almost unperturbed, however, considered in an ensemble with the Fe2, Fe1/1 and Fe1/2 centers represents fourth kind of the iron centers.

At low Fe2 iron concentrations (below 5 at.%), these plaquettes do not overlap (nearest Fe2 neighbor events have statistically low probability of the next order in the concentration), and we presented a spectroscopic evidence of the four magnetic centers model of iron centers in $\text{Fe}_{1.05}\text{Te}$.^[7] As the interstitial Fe2-type iron concentration increases, these plaquettes start to overlap, and at concentration of 12.5 at.%, being uniformly distributed, they do not leave a room for the third coordination ring around Fe2 centers. Our ab initio calculations of the electric-field gradients have shown that iron telluride $\text{Fe}_{1.125}\text{Te}$ contains three types of non-equivalent iron ion centers. One of them again consists of excess Fe2 iron ions. The other two groups at the first and second coordination rings (Fe1/1 and Fe1/2 groups, respectively) survive, however, against the case of

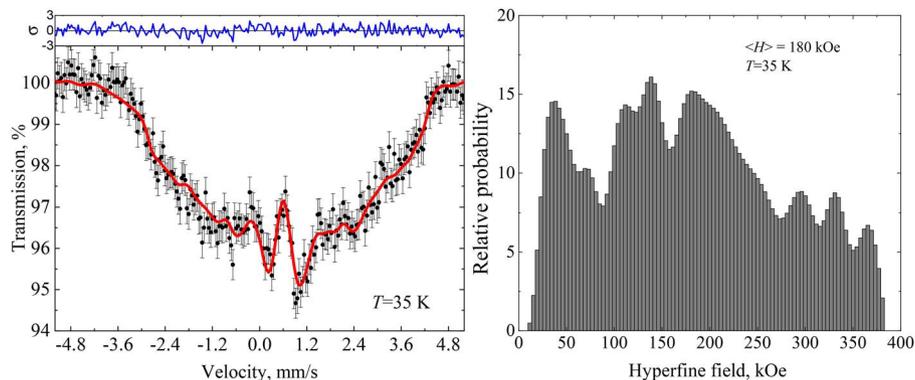


Figure 5. (Left) Mössbauer spectrum of the $\text{Fe}_{1.125}\text{Te}$ single crystalline sample obtained at 35 K and fitted by a distribution of hyperfine fields (shown in the right panel). The difference between the experimental and simulated spectra is shown by a thin blue line on top. (Right) The distribution of hyperfine fields.

Fe_{1.05}Te, the calculated electric field gradients at the Fe1/2 iron group is significantly reduced. It may be argued by the influence of neighboring Fe2 ions since the second coordination ring is common for the both Fe2 centers in average.

Indeed, using the three-center model of our Fe_{1.125}Te samples and ab initio calculated Mössbauer spectroscopy parameters for the fitting procedure, we have got good agreement between the model Mössbauer spectra and the experimental spectra measured at room temperature and different incidence angles of gamma-radiation. The low-temperature spectra were satisfactorily fitted by a set of magnetic sextets with a broad distribution of hyperfine fields within the assumption of incommensurate collinear SDW phase with the wave vector $q = 0.46 \pm 0.01$ realized in Fe_{1.125}Te according to the neutron scattering data of ref. [6].

For higher concentrations of excess Fe2 iron atoms, the plaquettes overlap so strongly that the interstitial iron ions Fe2 probably interact with each other via the common Fe1/1 iron ions of the first coordination ring. The proposed plaquette model is consistent with the physical picture following from the neutron diffraction studies^[6]: at low concentration of Fe2 atoms, strong magnetism of the interstitial iron leads to bicollinear antiferromagnetic order. The iron atoms Fe1 of the first coordination sphere around excess iron atoms Fe2 are ferromagnetically correlated, while the interaction between the Fe1 atoms is antiferromagnetic. In the case of strongly overlapping plaquettes at high Fe2 concentrations, the helical magnetic order realizes. The system Fe_{1.125}Te is at the border between the low and high concentration regimes, when, at uniform distribution, the plaquettes adjoin by the outer perimeter. This case is considered separately in ref. [6] and demonstrates collinear SDW.

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Conflict of Interest

The authors declare no conflict of interest.

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