01

Hysteresis of resistivity tensor in rare-earth polytellurides

© P.D. Grigoriev[1,2], A.A. Sinchenko[3,4], T.I. Mogilyuk[5], P.A. Vorobyov[2], D. Akparov[2], S.S. Alisultanov[6], A.M. Dyugaev[1]

[1] L.D. Landau Institute for Theoretical Physics, Chernogolovka, Russia
[2] National University of Science and Technology MISiS, Moscow, Russia
[3] Lomonosov Moscow State University, Moscow, Russia
[4] Kotelnikov Institute of Radio Engineering and Electronics, Russian Academy of Sciences, Moscow, Russia
[5] National Research Center „Kurchatov Institute", Moscow, Russia
[6] Amirkhanov Institute of Physics, Dagestan Federal Research Center, Russian Academy of Sciences, Makhachkala, Russia

E-mail: grigorev@itp.ac.ru

Received April 29, 2022
Revised April 29, 2022
Accepted May 12, 2022

Possible reasons for the temperature hysteresis of the Hall and diagonal components of resistivity tensor in tritellurides and tetratellurides of rare-earth metals, respectively, are analyzed. The width of this hysteresis exceeds 100 K in both families. This hysteresis is related to the charge density wave (CDW), but its detailed nature is still being discussed. It is known that it cannot be explained by a temperature variation in the CDW wave vector. In this paper, we discuss various interpretations of the observed hysteresis, present new experimental data showing a strong dependence of the hysteresis value on the temperature range, and propose new experiments (or a detailed analysis of unpublished data from existing ARPES measurements) that can substantiate or refute the proposed explanations for this unusual effect.

Keywords: charge density wave, hysteresis, conductivity, Hall coefficient, anisotropy.

DOI: 10.21883/PSS.2022.09.54142.23HH

1. Introduction

Tritellurides and tetratellurides of rare earth metals, RTe_3 and RTe_4, are highly anisotropic layered conductors. The Fermi surface (FS) in these compounds, according to band calculations and angle-resolved photoemission spectroscopy (ARPES) [1–5], consists of two pairs of corrugated sheets, perpendicular to each other and formed by p_x and p_y tellurium orbitals giving two bands α of electron spectrum. These sheets have an additional bilayer splitting corresponding to the even and odd z-wave function dependence in the tellurium binaries. The Fermi surface in the form of a corrugated sheet corresponds to the quasi-one-dimensional electron dispersion law $\epsilon_\alpha(k)$, well described in tight-binding approximation [1–3]. This latent, quasi-one-dimensional anisotropy and strong electron correlations result in a charge-density wave (CDW) [6] with a sufficiently high transition temperature T_{c1}, for most rare earth elements R T_{c1} above room temperature. This CDW transition and momentum dependence of the corresponding energy gap in the electron spectrum are clearly visible in ARPES [1,3–5] and in many other measurements [7–12]. Interestingly, the CDW transition is also accompanied by the disruption of conductivity isotropy along layers [12] as the system selects one CDW vector from two possible vectors, directed along the y axis. In RTe_3 compounds with heavier rare earth elements R = Dy, Ho, Er, Tm at a lower $T \leq T_{c2} \leq T_{c1}$ the second CDW with the wave vector $Q_2 \perp Q_1$ [7] occurs, which is already directed along the x axis. At very low temperatures of $T \lesssim 10$ K in RTe_3 there is also a series of magnetic transitions [13]. Under a pressure of RTe_3, the CDW disappears and superconductivity occurs [14], similar to many organic metals and high-temperature superconductors.

In the transition region to the second CDW, $\sim T_{c2}$, a strong temperature hysteresis of the Hall coefficient [15] is observed in rare earth trillurides RTe_3. The width of this hysteresis exceeds 100 K. In tetratellurides of rare earth metals RTe_4, there is an even stronger temperature hysteresis of the diagonal resistance component [3] with a width of about 200 K, which is probably a record one. Hysteresis often occurs when changing the CDW wave vector, because the CDW is pinned by defects of the crystal lattice [6]. However, there is no noticeable (greater than the measurement error) change in the CDW wave vector either in the tritellurides or in the tetratellurides, much less its hysteresis was detected [3,9,15–17]. Therefore, the

change of CDW wave vector was excluded from the possible hysteresis origins in all rare earth metals [3,15].

2. Experimental observations and hysteresis magnitude dependence on temperature change interval

Let's sum up briefly experimental observations of unusual hysteresis of electronic transport properties in rare earth metals.

In tritellurides, hysteresis is observed mainly in the Hall coefficient (see Fig. 1 in article [15] and Fig. 1 in this work), while in the diagonal component of the resistance tensor within the experimental error it is not noticeable (see Fig. 4, *b* and 4, *c* in Supplementary Information [16] to article [15]). As already noted, no temperature change in the CDW wave vector in tritellurides, much less its hysteresis, was detected in the X-ray scattering experiments [15–17,3] specifically performed for this purpose, which rules out the corresponding hysteresis scenario. The Hall resistance hysteresis was observed below the transition temperature to the second CDW and only in those RTe_3 compounds, where CDW_2 are present, in particular, in $ErTe_3$ and $HoTe_3$. The width of hysteresis is about 100 K. Fig. 1 presents new experimental data showing, in addition to the Hall coefficient hysteresis in $ErTe_3$ itself, a strong dependence of its value on the temperature change interval. If we do not go too low on temperature T, limiting ourselves to the $130\,\mathrm{K} < T < 175\,\mathrm{K}$ region, the value of hysteresis, that is, the difference of the Hall coefficient when heating and cooling, will decrease by an order of magnitude or even more.

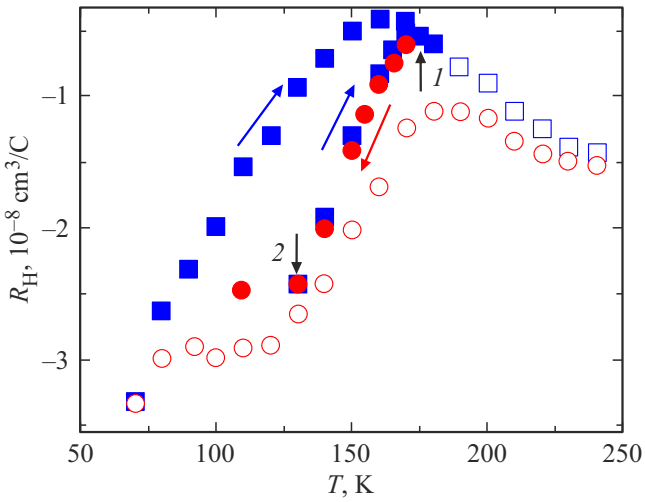

Figure 1. Temperature change of the Hall coefficient in $ErTe_3$ when heating from low T to *1*, corresponding to 175 K (blue squares), after cooling to *2* at $T = 130\,\mathrm{K}$ (red circles) and after warming up to point 1 (blue squares). Open blue squares and open red circles give a complete hysteresis cycle.

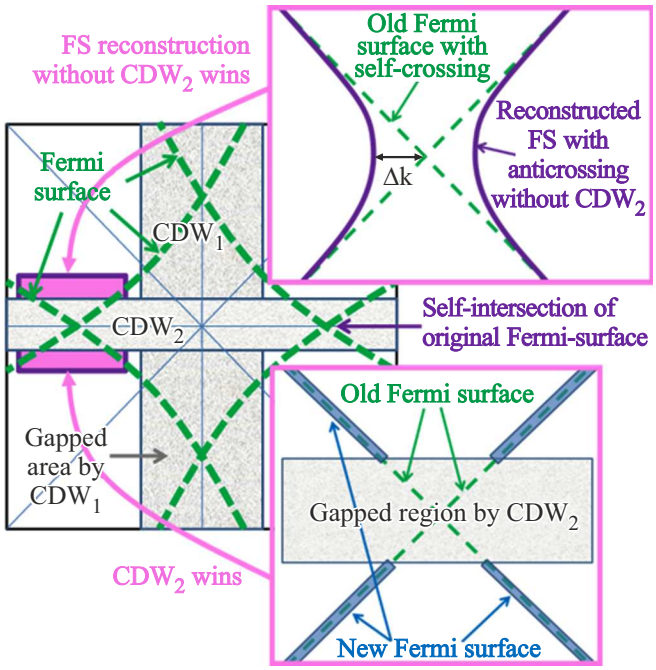

Figure 2. Schematic representation of the Fermi surface in rare-earth tritellurides and different scenarios of its reconstruction due to the second CDW_2 and due to band anticrossing in the area of their intersection at the Fermi level.

In tetratellurides, a similar hysteresis is observed in the diagonal component of the resistance tensor (see Fig. 2, *a* in [3]). The hysteresis width exceeds 200 K and appears to be a record in CDW materials. It should be noted that according to Fig. 3 of [3], in addition to the resistance hysteresis, the ARPES measurements also show an energy gap hysteresis at momentum $(k_x, k_y) \approx (\pm 0.57\pi/a, 0)$ (see Fig. 3, *a* of article [3]), and a similar hysteresis of X-ray scattering intensity on the CDW wave vector $Q_{CDW} \approx (0.2\pi/3b)$ (see Fig. 3, *b* of article [3]) is observed from the X-ray measurements. At the same temperature, these measured energy gaps and X-ray dissipation rates are higher when heated than when cooled. This corresponds to the fact that CDW is stronger at low temperature and competes with some other instability that is present even at a higher temperature. Unfortunately, article [3] does not contain data about the gap hysteresis at the point of $(0 \pm 0.57\pi/b)$ of the momentumd space symmetrical to the replacement of $x \to y$.

3. Effect Interpretations

Despite the apparent commonality of the effect, different physical explanations for this hysteresis of transport properties have been proposed in rare earth tritellurides and tetratellurides [15,3].

To explain the hysteresis of the Hall coefficient in rare earth tritellurides, the competition of two fundamentally different types of electronic ordering [15] was proposed:

(i) second CDW with wave vector $Q_2 \perp Q_1$ covering an appreciable Fermi-surface fraction by the gap $\Delta_2(k)$; and (ii) repulsion of degenerate levels with the formation of a local (in the momentum space near the intersection points of the Fermi surface from different bands) and large in the magnitude $V_0 > \Delta_2$ of gap at the Fermi level. The value of splitting of degenerate levels $V_0 > \Delta_1 > \Delta_2$, since unlike CDW, corresponds to the interaction at the zero wave vector and is summed with the hybridization of degenerate levels from due to overlapping of their wave functions. The system selects one of these two types of electronic ordering, each with its own energy gain. The estimates of this energy gain, given in article [15] show that they are of the same order, but the gain from CDW_2 is slightly higher because more electronic states are involved in the corresponding spectrum restructuring. Nevertheless, the repulsion of degenerate levels occurs even at high temperature, while CDW_2 occurs only at $T < T_{c2} \approx 100-200$ K. Therefore, when the temperature decreases, the CDW_2 arises against the background of splitting V_0. The calculation of the electronic susceptibility on the wave vector Q_2 showed [15] that the repulsion of levels at the intersection points of the Fermi surface does prevent the formation of CDW_2 because it reduces the Lindhardt susceptibility on the wave vector Q_2 (see Fig. 3 in [15]). Similarly, the CDW_2 reduces the energy gain from repulsion of levels at the intersection points of the Fermi surface, since the CDW_2 itself creates an energy gap in these regions of momentum space. Thus, depending on the temperature and the direction of its change (cooling or heating) one of these two types of electronic ordering is realized, which is schematically depicted in Fig. 2.

To explain the hysteresis of resistance in tetratellurides of rare earth metals, a different model was proposed [3]. To do this, CDW interactions are introduced on different tellurium layers. In tetratellurides there are three different layers with the numbers $i = 0, 1, 2$. CDW modulates the electron density ρ_i on each layer with an amplitude u_i: $\tilde{\rho}_i = u_i \cos(Qr + \phi_i)$.

CDW on different layers is bound by the Coulomb interaction and through phonons. This interaction is quite strong, so that article [3] reasonably assumes that the relative phase shift of the CDW within each bilayer $\phi_1 - \phi_2$ is fixed at an energy scale significantly larger than those under consideration. Further in [3] the phase difference of CDW $\phi \equiv \phi_1 - \phi_0$ between the bilayer and tellurium monolayer in rare earth tetratellurides is examined. The ordinary Coulomb interaction or interaction through polarization of the medium (phonons) gives bilinear interaction terms $u_0 u_1^* + c.c. \propto \cos\phi$, but next orders of perturbation theory can also give biquadratic terms $(u_0 u_1^* + c.c.)^2 \propto \cos^2\phi$. Therefore, in [3] the decomposition of free energy by $\cos\phi$ is introduced:

$$F(\phi) = F_0 + a\cos\phi + b\cos^2\phi. \qquad (1)$$

At $|a/b| < 2$ there are two free energy minima, and article [3] suggests that the observed hysteresis is due to a first-order phase transition between these two free energy minima.

In our view, this second scenario of hysteresis is unlikely. First, it requires [3] that the free energy decomposition coefficients satisfy $a \sim b$, and preferably even $a < b$, which means a random almost complete cancellation of the Coulomb and phonon interaction contributions of the CDW in the main order. This accidental cancellation in a very wide temperature range is unlikely. Second, this interpretation essentially relies [3] on the assumption that such hysteresis is observed only in tetratellurides, which have tellurium monolayers in addition to bilayers, and that hysteresis should be absent in tritellurides, which have no such monolayers. However, as shown in [15] and above in Fig. 1, this is not the case, and there is a comparable width of hysteresis in tritellurides. The likelihood of a similar accidental cancellation in the contributions of Coulomb and phonon interactions within tellurium bilayer with a layer spacing of about 3 Å is very low. Third, even assuming two minima in the free energy (1), it is not clear why this should lead to such a broad (in temperature) phase transition. At the same time, the hysteresis width calculated in the first scenario as the difference between the instability temperature of CDW_2 in the presence of and without repulsion of the levels at the intersection points of FS, agrees well with experiment [15]. Fourth, given that the energy gain of CDW [6]:

$$\Delta E_{CDW} \approx \sum_{\alpha} \int d^3k \delta\big(\epsilon_\alpha(k) - E_F\big)\Delta^2_{CDW}(k,\alpha)/2, \qquad (2)$$

where k, α — is the momentum and electron band number numbering their quantum state. The noticeable difference in the gap $\sim 20\%$ size, determined by the direction of temperature change, must lead to a significant difference in the energy of the CDW and compensated by some-some other energy. In the first scenario, this is an energy gain from level repulsion [15] $\Delta E_{V_0} \propto V_0^n$, unrelated to CDW. Here the exponent of degree $n = 3$ as opposed to the usual $n = 2$ from the majority of instabilities. An additional degree V_0 occurs because the width of the electron spectrum restructuring region along the Fermi surface is also small by the parameter V_0/E_F [15]. In the second scenario [3] it is not clear how the energy difference of the CDW in equation (2) is compensated. The interaction between the CDWs on the different tellurium layers is already embedded in the size of the CDW gap. It is also possible to redistribute the gap size along the Fermi surface or between the α bands, i.e., to change the $\Delta^2_{CDW}(k,\alpha)$ dependence, and such redistribution can in principle be detected by analyzing the ARPES data in detail. Fifth, the strong dependence of the hysteresis value on the temperature change interval shown in Fig. 1 agrees well with the first scenario. Indeed, if temperature is not sufficiently low, when the second CDW is already established, the repulsion of levels in the area of their intersection (anti-crossings) will not break, and hysteresis will be very weak. In the second scenario, a broad phase

transition of the first kind would seem to lead to wide hysteresis even if not to fall low enough at the temperature.

4. Discussion of possible further experimental confirmations and conclusions

The interaction or competition of different types of electronic instability is quite common in highly correlated electronic systems, including high-temperature superconductors, and is certainly of great scientific interest. In rare earth metal polytellurides this interaction leads to a new interesting effect — strong temperature hysteresis of electron-transport properties, whose width exceeds 100 K. So far, there is no clear explanation for this effect. The distinguishing feature of the electron structure of polytellurides of rare earth metals is the intersection of electronic levels originating from different bands at the Fermi level with the same quasi-momentum value. We suggest that the hysteresis observed in tri- and tetratelluirides is of the same nature. Some differences, for example, the fact that in tritellurides hysteresis is observed mainly in the Hall coefficient, and in tetratelluirides in the diagonal resistance component, can easily be explained by the fact that in tritellurides, the CDW does not cover the entire Fermi surface with an energy gap, while in tetratelluirides, the CDW gap completely covers the Fermi surface. Therefore, in tetratellurides, the variation of the CDW gap size, especially near its minimum, has an exponentially large impact on the diagonal component of the electrical resistance. In tritellurides, metallic conductivity is maintained and the Hall effect can be observed, but the change in the size of the CDW gap does not significantly affect the conductivity, since the contribution to the diagonal conductivity from states under the CDW is bypassed by a contribution from metal (gapless) electronic states.

According to our proposed model [15] this hysteresis arises from the competition of energy winnings from the CDW and from the for pushing off levels associated with the intersection of electronic bands. An alternative scenario proposed in the work [3] is a very wide phase transition of the first kind between two CDW space configurations, differing by the relative phase shift of the CDW on different tellurium layers, for example, on bilayers and monolayers.

Detailed ARPES measurements data can confirm or prove wrong any of the proposed resistance tensor hysteresis scenarios. To do this, it would be very useful to know the size of the gap in the electron spectrum at the Fermi level symmetrically relative to the replacement of $x \to y$ intersection points on the Fermi surface during heating and cooling. If the proposed scenario is implemented, then, first, at these points of the momentum space during cooling, the size of this gap will be significantly larger than the average gap of the CDW, since its nature is not related to the CDW, but to repulsion of degenerate levels. Second, the difference in the size of this gap in the cooling and heating band intersection will be opposite to the gap difference in other areas of the momentum space, as it is not formed by CDW, but on the contrary competes with CDW.

Further study of magnetoresistance in polytellurides of rare earth metals can also help to confirm or prove wrong some scenario of the resistance tensor hysteresis. For example, the observation of a linear magneto-resistance [18,19] in rare earth metal tritellurides points to the so-called „hotspots“ on the Fermi surfacei, which amplify the electron dissipation due to CDW volatility or due to intersecting bands. If we could observe magnetic quantum oscillations in the temperature interval of hysteresis, which is possible in principle, since rare earth metal tritellurides have little effective electron mass, this would shed light on the restructuring of the Fermi surface, caused by the formation of the second CDW.

It is also worth noting the possibility of indirectly experimental confirmation of the spatial phase separation, often associated with phase transitions of the first kind, on the temperature dependence of resistance anisotropy. The conductivity theory in heterogeneous materials [20], applied to highly anisotropic materials [21–26], indicates a specific dependence of resistance anisotropy, which can give information about the approximate shape and size of the islets of one phase in the matrix of the other, for example, metal or any well-conducting phase in the material with CDW.

Funding

T.I. Mogilyuk thanks RFFI for the financial support (grant No. 21-52- 12027). P.D. Grigoriev thanks for RFFI grant 21-52-12043. Z.Z. Alisultanov thanks for grant of the RF President MD-647.2020.2. A.M. Dyugaev thanks for the state task 0033-2019-0001 „Development of the theory of condensed matter“. A.A. Shinchenko thanks for the state task IRE RAN. D. Akparov thanks the „BASIS“ Foundation grant #22-1-1-24-1.

Conflict of interest

The authors declare that they have no conflict of interest.

References

[1] V. Brouet, W.L. Yang, X.J. Zhou, Z. Hussain, R.G. Moore, R. He, D.H. Lu, Z.X. Shen, J. Laverock, S.B. Dugdale, N. Ru, I.R. Fisher. Phys. Rev. B **77**, 235104 (2008).

[2] D. Wu, Q.M. Liu, S.L. Chen, G.Y. Zhong, J. Su, L.Y. Shi, L. Tong, G. Xu, P. Gao, N. L. Wang. Phys. Rev. Mater. **3**, 024002 (2019).

[3] B.Q. Lv, Alfred Zong, D. Wu, A.V. Rozhkov, B.V. Fine, Su-Di Chen, Makoto Hashimoto, Dong-Hui Lu, M. Li, Y.-B. Huang, J.P.C. Ruff, D.A. Walko, Z.H. Chen, Inhui Hwang, Yifan Su, Xiaozhe Shen, Xirui Wang, Fei Han, Hoi Chun Po, Yao Wang, Pablo Jarillo-Herrero, Xijie Wang, Hua Zhou, Cheng-Jun Sun, Haidan Wen, Zhi-Xun Shen, N.L. Wang. Nuh Gedik. Phys. Rev. Lett. **128**, 036401 (2022).

[4] R.G. Moore, V. Brouet, R. He, D.H. Lu, N. Ru, J.-H. Chu, I.R. Fisher, Z.- X. Shen. Phys. Rev. B **81**, 073102 (2010).
[5] F. Schmitt, P.S. Kirchmann, U. Bovensiepen, R.G. Moore, J.-H. Chu, D.H. Lu, L. Rettig, M. Wolf, I.R. Fisher, Z.-X. Shen. New J. Physics **13**, 063022 (2011).
[6] G. Grüner. Density waves in Solids. 1st ed. Perseus Publishing (2000).
[7] N. Ru, C.L. Condron, G.Y. Margulis, K.Y. Shin, J. Laverock, S.B. Dugdale, M.F. Toney, I.R. Fisher. Phys. Rev. B **77**, 035114 (2008).
[8] A. Fang, N. Ru, I.R. Fisher, A. Kapitulnik. Phys. Rev. Lett. **99**, 046401 (2007).
[9] M. Lavagnini, M. Baldini, A. Sacchetti, D. Di Castro, B. Delley, R. Monnier, J.-H. Chu, N. Ru, I.R. Fisher, P. Postorino, L. Degiorgi. Phys. Rev. B **81**, 081101(R) (2010).
[10] A. Banerjee, Yejun Feng, D.M. Silevitch, Jiyang Wang, J.C. Lang, H.-H. Kuo, I. R. Fisher, T.F. Rosenbaum. Phys. Rev. B **87**, 155131 (2013).
[11] B.F. Hu, B. Cheng, R.H. Yuan, T. Dong, N.L. Wang. Phys. Rev. B **90**, 085105 (2014).
[12] A.A. Sinchenko, P.D. Grigoriev, P. Lejay, P. Monceau. Phys. Rev. Lett. **112**, 036601 (2014).
[13] N. Ru, J.-H. Chu, I.R. Fisher. Phys. Rev. B **78**, 012410 (2008).
[14] D.A. Zocco, J.J. Hamlin, K. Grube, J.-H. Chu, H.-H. Kuo, I.R. Fisher, M.B. Maple. Phys. Rev. B **91**, 205114 (2015).
[15] P.D. Grigoriev, A.A. Sinchenko, P.A. Vorobyev, A. Hadj-Azzem, P. Lejay, A. Bosak, P. Monceau. Phys. Rev. B **100**, 081109(R) (2019). [DOI: 10.1103/PhysRevB.100.081109].
[16] P.D. Grigoriev, A.A. Sinchenko, P.A. Vorobyev, A. Hadj-Azzem, P. Lejay, A. Bosak, P. Monceau. Supplementary Materials Ref. [15] http://link.aps.org/supplemental/10.1103/PhysRevB.100.081109 [see also arXiv:1906.11125].
[17] A. Girard, T. Nguyen-Thanh, S.M. Souliou, M. Stekiel, W. Morgenroth, L. Paolasini, A. Minelli, D. Gambetti, B. Winkler, A. Bosak. J. Synchrotron Rad. **26**, 272 (2019).
[18] A.A. Sinchenko, P.D. Grigoriev, P. Lejay, P. Monceau. Phys. Rev. B **96**, 245129 (2017).
[19] A.V. Frolov, A.P. Orlov, P.D. Grigoriev, V.N. Zverev, A.A. Sinchenko, P. Monceau. JETP Lett. **107**, 324 (2018).
[20] S. Torquato. Random heterogeneous materials: microstructure and macroscopic properties. Springer-Verlag, N. Y.(2002).
[21] A.A. Sinchenko, P.D. Grigoriev, A.P. Orlov, A.V. Frolov, A. Shakin, D.A. Chareev, O.S. Volkova, A.N. Vasiliev. Phys. Rev. B **95**, 165120 (2017).
[22] P.D. Grigoriev, A.A. Sinchenko, K.K. Kesharpu, A. Shakin, T.I. Mogilyuk, A.P. Orlov, A.V. Frolov, D.S. Lyubshin, D.A. Chareev, O.S. Volkova, A.N. Vasiliev. JETP Lett. **105**, 786 (2017).
[23] S.S. Seidov, K.K. Kesharpu, P.I. Karpov, P.D. Grigoriev. Phys. Rev. B **98**, 014515 (2018).
[24] T.I. Mogilyuk, P.D. Grigoriev, K.K. Kesharpu, I.A. Kolesnikov, A.A. Sinchenko, A.V. Frolov, A.P. Orlov. FTT **61**, *9*, 1599 (2019) (in Russian). [T.I. Mogilyuk, P.D. Grigoriev, K.K. Kesharpu, I.A. Kolesnikov, A.A. Sinchenko, A.V. Frolov, A.P. Orlov. Phys. Solid State **61**, 1549 (2019)].
[25] K.K. Kesharpu, V.D. Kochev, P.D. Grigoriev. Crystals **11**, 72 (2021).
[26] V.D. Kochev, K.K. Kesharpu, P.D. Grigoriev. Phys. Rev. B **103**, 014519 (2021).