Investigation of the phonon dispersion associated with superlattice reflections in the BiS₂-based superconductor LaBiS₂O_{0.5}F_{0.5}

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The phonon dispersion of a BiS₂-based superconductor LaBiS₂O_{0.5}F_{0.5} is investigated by first-principles calculations and inelastic x-ray scattering experiments. The origin of superlattice (SL) reflections arising from transverse-type lattice modulation, which were recently reported in [J. Kajitani *et al.*, J. Phys. Soc. Jpn. **90**, 103601 (2021)], is discussed in terms of lattice dynamics. Our first-principles calculations of phonon dispersion and the Fermi surfaces (FSs) demonstrate that the phonon mode corresponding to the transverse-type lattice modulation is unstable, and the propagation vector corresponding to the SL reflections is close to the FS nesting vector, which suggests that the phonon softening originates from the FS nesting. Against these calculated expectations, measured phonon dispersion in LaBiS₂O_{0.5}F_{0.5} along the Z-A direction, where the SL point is located, shows no remarkable temperature dependence, and there are no steeply declining branches accompanied with a softening around the SL point. Based on these results, we discuss the two possibilities for the transverse lattice modulation in LaBiS₂O_{0.5}F_{0.5}: the order-disorder-type structural transition and the displacive structural transition with an overdamped mode, for both of which the local structure distortion or the short-range correlation within the BiS₂ plane would be essential.

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I. INTRODUCTION

BiS₂-based superconductors (SCs) have attracted considerable interest as a new family of layered superconducting compounds [1-3], after the well-studied cuprates [4], MgB₂ [5], and iron-based SCs [6]. The new systems show similar features, especially the cuprates and iron-based SCs. In the representative parent compound LaBiS₂O, for example, superconductivity is made to emerge by substituting O^{2-} to F^{-} [7–9]. Electronic band structure calculations for LaBiS₂O_{1-x} F_x demonstrated that the quasi-one-dimensional Fermi surfaces (FS) composed of Bi-6p and S-3p orbitals have a good nesting condition at the wave vector (π, π) [10]. By analogy with cuprates and iron-based SCs, an unconventional pairing mechanism related to the FS nesting is expected [11,12]. Indeed, several experiments have suggested the importance of the FS nesting to superconductivity in BiS_2 -based SCs [13–15]. On the other hand, the calculated electron-phonon coupling constant is quite large [16,17]. This large coupling constant well reproduces the experimental value of the largest transition temperature, T_c , of 2.5 K in the optimally doped composition LaBiS₂O_{0.5}F_{0.5} within the conventional Bardeen-Cooper-Schrieffer scheme [16,17]. Although the annealing process for LaBiS₂O_{0.5}F_{0.5} under the

high pressure of 2 GPa increases T_c up to 10.2 K [7], even this value can be explained by the large electron-phonon coupling constant [16,17]. The pairing mechanism in BiS₂-based SCs is still under debate.

Much attention has been paid to the relationship between a crystal structure and lattice dynamics in LaBiS₂O_{1-x}F_x, which is significant for the viewpoints of dielectricity [18] and thermoelectricity [19], as well as the lattice instability possibly connected with a pairing mechanism. Yildirim showed that imaginary phonon modes appear at the Γ point in nondoped LaBiS₂O, using first-principles calculations [18]. These imaginary phonon modes are associated with a shift of in-plane S1 atoms along the *a* axis (see Fig. 1), which lowers the symmetry from *P4/nmm* to polar monoclinic space groups [18]. Subsequently, precise crystal structure analyses using a single crystal have confirmed the expected shift of in-plane S atoms along the *a* axis and revealed that the space group of LaBiS₂O at room temperature is monoclinic *P2*₁/*m* [20].

On the other hand, for the optimally doped composition x = 0.5 ($T_c \sim 2.5$ K [7]), imaginary phonon modes appear around the M point [16,18]. Nevertheless, it has been reported that LaBiS₂O_{0.5}F_{0.5} does not show symmetry lowering and keeps the space group *P*4/*nmm* at room temperature [21]. Recently, superlattice (SL) reflections with the propagation vector $q_{SL} = (\zeta, \zeta, 0.5; \zeta \simeq 0.207)$ were observed below ~260 K in the x = 0.5 sample, which differs

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FIG. 1. Crystal structure of $LaBiS_2O_{0.5}F_{0.5}$. The rectangle indicates the unit cell. The image of the crystal structure is generated using the VESTA software developed by Monma and Izumi [24].

from the symmetry lowering of LaBiS₂O [21]. Kajitani *et al.* have revealed that these SL reflections arise from an in-plane transverse-type lattice modulation and they have discussed the possibility that a checkerboard charge density wave (CDW) with $q_{CDW} = (2\zeta, 2\zeta, 0)$ concomitantly occurs [21]. Because q_{CDW} is close to the FS nesting vector predicted, they have also suggested that the CDW state originates from the Peierls instability [21]. Similar SL reflections are observed in NdBiS₂O_{1-x}F_x [22].

A CDW generally tends to be coupled with a longitudinal lattice modulation and their wave numbers are usually common [23], while the lattice modulation in LaBiS₂O_{0.5}F_{0.5} is transverse type and is characterized by q_{SL} , not q_{CDW} [21]. Therefore, the transverse-type lattice modulation in LaBiS₂O_{0.5}F_{0.5} possibly differs from a usual CDW state. To gain a constructive insight into the transverse-type lattice modulation in LaBiS₂O_{0.5}F_{0.5}, it is helpful to examine lattice dynamics and its temperature dependence such as a soft phonon mode concomitant with the SL reflections.

In this study, we use first-principles calculations and an inelastic x-ray scattering (IXS) technique to investigate phonon dispersion in LaBiS₂O_{0.5}F_{0.5} to shed light on the origin of the SL reflections. Our first-principles calculations show that the phonon mode corresponding to the transverse-type lattice modulation is unstable, suggesting that phonon softening may originate from the FS nesting. However, we observe that phonon dispersion in LaBiS₂O_{0.5}F_{0.5} along the Z-A direction is unchanged with changing temperature, and there are no soft modes around q_{SL} . To explain these results, we propose two possibilities for the characteristic nature of the transverse lattice modulation in LaBiS₂O_{0.5}F_{0.5}.

II. CALCULATIONS AND EXPERIMENTS

Electronic states and phonon dispersions of $\text{LaBiS}_2\text{O}_{1-x}\text{F}_x$ were calculated using the ABINIT package [26,27], which is based on the pseudopotential method with the plane-wave basis set and density functional theory. The plane-wave cutoff energy was 952 eV, and the k-point mesh on the $16 \times 16 \times 4$ Monkhost-Pack grid [28] was used. For the exchangecorrelation functional, the local density approximation (LDA) parametrized by Perdew and Wang [29] was adapted. Since the F-doped materials are metals, the occupations of the one-electronic states are broadened by the Fermi-Dirac distribution with T = 316 K. This temperature is low enough to see the soft modes due to the nesting of the Fermi surfaces. The Troullier-Martins pseudopotentials [30] are generated by the FHI98PP program [31]. The lattice constants in the calculations are set to be the experimental values (a = 4.0585 Å and c = 13.324 Å), and the atomic positions are optimized by the Broyden-Fletcher-Goldfarb-Shanno algorithm [32], until the forces are lower than 0.0026 eV/Å. The interatomic interactions to obtain phonon dispersions are obtained by the density functional perturbation theory (DFPT) [33,34]. The dynamical matrix is calculated on the $4\sqrt{2} \times 4\sqrt{2} \times 2$ grid in the reciprocal space, which is the reciprocal lattice of the $4\sqrt{2}a \times 4\sqrt{2}a \times 2c$ superlattice. We need to use a fine grid along [110] directions to elucidate the incommensurate soft modes. The F-doping is simulated by the virtual crystal approximation, which uses an arithmetic mean value of the pseudopotentials of O and F with the mixing ratio x. The IXS spectra are simulated with the calculated phonon modes according to the method given in the Supplemental Material of Ref. [35].

A single crystal of LaBiS₂O_{0.5}F_{0.5} ($T_c \sim 2.5$ K) is identical to the one used in the previous study [21]. The concentration of F is estimated by the reported x dependence of the lattice constants [7,36]. Before the IXS experiments, we performed a synchrotron radiation x-ray diffraction experiment with large cylindrical image-plate diffractometers to confirm that the sample used in this study is a single-domain crystal. This synchrotron radiation x-ray diffraction experiment was conducted at BL-8A, Photon Factory (PF), at High Energy Accelerator Research Organization, Tsukuba, Japan.

The IXS experiments were carried out at BL35XU of SPring-8 in Japan [37]. The incident x-ray energy was tuned to 21.747 keV with an energy resolution of 1.5 meV, using a Si(11 11 11) backscattering. In reciprocal lattice units, the resolution of a momentum transfer was set to (0.06, 0.06, 0.06) for longitudinal and [110] transverse measurements and to (0.04, 0.05, 0.06) for [001] transverse measurements. The sample temperature was controlled by a He closed-cycle refrigerator. The phonon energies were obtained by fitting the measured IXS spectra using the Lorentz function with the Bose factor [38]. Because the sample was mounted on a sapphire plate in the IXS experiments, we also measured the IXS spectra from only the sapphire plate for the background estimation.

III. RESULTS

The blue "bare" curve in Fig. 2(b) shows the phonon dispersion of $LaBiS_2O_{0.5}F_{0.5}$ obtained from DFPT. In this figure, imaginary frequencies of phonon energies are conventionally plotted as the dispersion curves with minus signs, where the magnitude of imaginary frequencies indicates the structural instability. Several imaginary modes exist, and the lowest



FIG. 2. (a) Schematic Brillouin zone of LaBiS₂O_{0.5}F_{0.5} with high-symmetry points. SL shows a reciprocal lattice point where the superlattice reflection appears below ~ 260 K (see the main text for detail). For visibility, the c^* axis is elongated. Calculated phonon dispersion of (b) LaBiS₂O_{0.5}F_{0.5} and of (c) LaBiS₂O_{0.8}F_{0.2}. In the calculation, a tetragonal unit cell (*P4/nmm*) is employed. Red curves in panels (b) and (c) are "modified" phonon dispersions for the soft modes to have very small real frequencies, to confirm whether the soft mode actually exists by comparing with the experimental results (see the main text and the Supplemental Material [25] for more detail).

energy mode is a transverse mode with the propagation vector of (~0.35, ~0.35, 0.5) located on the Z-A line. This phonon mode is associated with a vibration of S1 atoms residing in the BiS₂ plane (see Fig. 1) and, therefore, corresponds to the reported in-plane transverse-type lattice modulation. As shown in Fig. S1 in the Supplemental Material [25], this propagation vector is close to the nesting vector. This suggests that the FS nesting is responsible for the aforesaid phonon softening. However, the propagation vector of the most unstable phonon disagrees with $q_{SL} = (\zeta, \zeta, 0.5; \zeta \simeq 0.207)$. In our calculation, phonon dispersion and the propagation vectors of the soft modes highly depend on calculation conditions such as the k-point mesh and approximations to density functionals (e.g., LDA or the generalized gradient approximation). This may be partly because a van Hove singularity is close to the Fermi energy in the vicinity of x = 0.5, as several studies have suggested [10,39–42]. Therefore, strict comparison between the experimental and calculated phonon dispersions seems to be difficult in this system.

To construct a model that reproduces the value of q_{SL} and phonon dispersion in our calculation condition, we examine FSs of x = 0.1, 0.2, 0.3, 0.4, and 0.5 in LaBiS₂O_{1-x}F_x. As a result, we find that FS of x = 0.2 has a good nesting condition at (~0.2, ~0.2, 0.5), which is close to $q_{\rm SL}$ (Fig. S1 in the Supplemental Material [25]). Figure 2(c) shows the calculated phonon dispersion of LaBiS₂O_{0.8}F_{0.2}. Several imaginary modes occur, as in the case of x = 0.5, with the most unstable mode located around (0.2, 0.2, 0.5). These results suggest that the phonon softening at x = 0.2 originates from the FS nesting. The lowest energy mode of x = 0.2 is the transverse mode associated with the vibration of S1 atoms residing in the BiS₂ plane, as in the case of x = 0.5. In addition, as is shown later, the calculation results of the phonon dispersion for x = 0.2 reproduce the experimental results better than those for x = 0.5 as well as q_{SL} .

Our calculation also indicates that q_{SL} depends on x and is located on the Z-A line. This x dependence of q_{SL} (or q_{CDW}) is consistent with the results observed in NdBiS₂O_{1-x}F_x [22]. Therefore, our calculation seems to well capture overall phonon features, at least q_{SL} and phonon dispersion, and their x dependence, although x in the calculation does not coincide with the actual concentration x. Thus, we adopt the calculated results of x = 0.2 as our model and use them for comparing with our experimental results.

Note that, by the angle-resolved photoemission spectroscopy of $RBiS_2O_{1-x}F_x$ (R = rare-earth elements) single crystals, the actual electron doping level estimated from the size of the FS tends to become smaller than x of the nominal composition [39–41]. For example, the size of the FS in NdBiS₂O_{0.5}F_{0.5} indicates the electron doping of x = 0.16 [39]. This shift in x agrees well with that of the present study. Although some possible origins for the shift have been proposed, e.g., Bi ion deficiency and/or F ion trapping in interstitial sites, their quantitative influences are still unclear and remain to be elucidated further.

The negative energies in the "bare" phonon dispersions shown in Figs. 2(b) and 2(c) are those of soft modes. Such soft modes are not displayed in IXS spectra, since they are not oscillations with real frequencies. The soft modes show large temperature dependence of energy. The energies will become very small around the transition temperature if the transition is a displacement-type structural transition. Therefore, to confirm whether the soft mode actually exists by comparing with the experimental results, the phonon dispersions are modified for the soft modes to have very small real frequencies. In this modification, we alter the values of the interatomic force constants (the dynamical matrix) obtained by DFPT, so that only phonon energies of the soft modes become positive without change in atomic displacements of the soft modes. The energies and atomic displacements for the other modes are almost not affected. For additional details on the modification methods, refer to the Supplemental Material [25]. These modified dispersions are shown in Figs. 2(b) and 2(c) by the red curves.

Based on the calculation results, we focus on the phonon dispersion along the Z-A direction and its temperature dependence. Figures 3(a)-3(c) (left panels) show the measured dynamical structure factor of LaBiS₂O_{0.5}F_{0.5} as a function of momentum transfer in reciprocal lattice units (r.l.u.) and energy (*E*) transfer in meV for three polarization geometries along the Z-A direction at room temperature. A propagation vector of phonon q is $(q, \pm q, 1/2)$. In this study, we use pseudo notations for (a) longitudinal $e \parallel [110]$ geometry, (b) transverse $e \parallel [1\overline{10}]$ geometry, and (c) transverse $e \parallel [001]$ geometry, respectively, where e is a polarization vector of a vibration.

The middle and right panels of Fig. 3 are the calculated (modified) dynamical structure factors for x = 0.2 and x = 0.5, respectively. Except for the contribution of the several unstable modes, the calculation results for x = 0.2 reproduce the experimental results better than those for x = 0.5. For example, in the calculated dynamical structure factor of x = 0.5 for the transverse $e \parallel [001]$ geometry [Fig. 3(c)], there are two modes with relatively high intensities ($E = \sim 8.2$ and 10 meV) at the zone boundary, while in that of x = 0.2, only one mode (E = 8 meV) can be seen at the zone boundary, which is consistent with the observation. Moreover, as stated below in more detail, the observed tiny signals in the transverse $e \parallel [1\overline{10}]$ geometry [Fig. 3(b)] seem to be well captured by the calculation results for x = 0.2.

We analyze the IXS spectra by using the Lorentz function with the Bose factor to more accurately determine the phonon energies. Figure 4 shows the observed and calculated IXS spectra as a function of *E* for the transverse $e \parallel [1\overline{1}0]$ geometry (the fitting results of the longitudinal $e \parallel [110]$ and the transverse $e \parallel [001]$ geometries are shown in the Supplemental Material [25]). The q dependence of the two modes determined by the fitting procedure (black arrows) agrees well with the calculation, except for the slight difference of the values of E. Small peaks seen in the calculated IXS spectra, especially around (q, E) = (0.335 r.l.u., 10 meV) [Fig. 4(g)] and (q, E) = (0.495 r.l.u., 8 meV) [Fig. 4(f)], also explain the observed tiny signals and broadening of high-intensity peaks [Figs. 4(a) and 4(b)], although these tiny signals could not be determined by the fitting due to the insufficient resolution. On the other hand, the unstable modes predicted by our calculation (orange arrows) cannot be seen in the experimental result around q = 0.207. Obviously, a phonon peak at E = 4.5 meV in the experiment is not broadened and is not asymmetric.

To reveal whether soft modes corresponding to the SL reflection exist or not, we investigated the temperature dependence of the IXS spectrum at the SL point in the vicinity of the phase transition temperature $T^* \sim 260$ K. Figure 5(a) shows the temperature dependence of IXS spectra around the SL point in the [110] transverse geometry. This clearly demonstrates that the predicted soft modes do not appear in the finite energy transfer region ($E \neq 0$) even with decreasing temperature toward and through the structural transition. As shown in the inset in Fig. 5(a), the energy of the lowest



FIG. 3. Dynamical structure factors of LaBiS₂O_{1-x}F_x at room temperature for (a) longitudinal $e \parallel [110]$ geometry, (b) transverse $e \parallel [1\overline{1}0]$ geometry, and (c) transverse $e \parallel [001]$ geometry, respectively, where e is a polarization vector of a vibration. Left panels: measured dynamical structure factor of LaBiS₂O_{0.5}F_{0.5}. White circles are peak positions of spectra obtained by the fitting analyses. Middle and right panels: calculated dynamical structure factors for x = 0.2 and x = 0.5, respectively. To compare with the experimental results, the calculated dynamical structure factors are modified. For clarity, the color gauge showing the strength of intensity is adjusted in each panel.



FIG. 4. [(a)–(e)] Measured IXS spectra of LaBiS₂O_{0.5}F_{0.5} along the Z-A direction at room temperature. Data were obtained in the transverse $e \parallel [1\overline{10}]$ geometry, where e is a polarization vector of a vibration. Black arrows indicate peak positions of each phonon excitation obtained by the fitting analyses. [(f)–(j)] Calculated IXS spectra of LaBiS₂O_{0.8}F_{0.2} for the same mode as in panels (a)–(e) at room temperature (we compare the experimental data of x = 0.5 with the calculation results of our model). Note that the minus sides of IXS spectra indicate the anti-Stokes scatterings, which entirely differ from the minus side of Fig. 2, because the phonon modes on the minus side in Fig. 2 are not observable vibration modes. Black and orange arrows indicate the identical peaks measured by the experiments and the predicted peaks of the soft modes.

phonon excitation (\sim 4.5 meV) around the SL point does not decrease over the transition temperature 260 K, although the peak is overlapped by the developing superlattice reflection at low temperatures (a reduction in its intensity is due to the Bose factor). Moreover, changes in the phonon energies are not observed in the longitudinal [Fig. 5(b)] and the [001] transverse [Fig. 5(c)] geometries. These results indicate that there are no steeply declining branches accompanied with the predicted instability around the SL point.

We also mention the temperature dependence of the elastic scattering (centered on E = 0 meV) at the SL point. As shown in Fig. 5(a), the intensity of the elastic scattering in the [110] transverse geometry drastically increases with decreasing temperature. The integrated intensity of this elastic scattering shows an order-parameter-like temperature dependence that starts to increase at ~260 K [Fig. 5(d)]. In the longitudinal [Fig. 5(b)] and the [001] transverse [Fig. 5(c)] geometries, in contrast, the intensities of the elastic scatterings show almost no change, except for the slight increases at low temperatures, which are probably due to difference of the Debye-Waller factor. These results are consistent with the previously reported reflection condition for the SL reflection [21]. We add that the calculated soft modes satisfy the reflection condition for the SL reflection.

Note that the convolution with a resolution function in the experiments possibly makes it hard to observe the soft modes. However, this possibility is ruled out, as shown in Fig. S3 in the Supplemental Material [25].

In Fig. 6, the phonon energies obtained by the fitting analyses are summarized as phonon dispersion along the Z-A direction at the selected temperatures. We find that phonon dispersion along the Z-A direction shows no



FIG. 5. Temperature dependence of IXS spectra at (a) (3.207, 2.792, 0.501), (b) (3.207, 3.206, 0.499), and (c) (0.200, -0.201, 16.495). The inset in panel (a) shows the temperature dependence of a phonon peak position around 4.5 meV [indicated by a black arrow in panel (a)]. (d) Integrated intensities of the elastic components for the three polarizations as a function of temperature.

remarkable temperature dependence, and the line widths of each phonon spectra do not show drastic changes even at the SL point (not shown).

IV. DISCUSSION

Here, we consider the characteristic nature of the transverse lattice modulation in LaBiS₂O_{0.5}F_{0.5}. According to our calculations, the lattice instability leading to the transverse lattice distortion at $T^* \sim 260$ K is due to the FS nesting. Although the usual CDW transition due to the FS nesting is generally accompanied with a soft mode, no soft modes corresponding to the lattice instability are observed in our



FIG. 6. Measured phonon dispersion of $LaBiS_2O_{0.5}F_{0.5}$ along the Z-A direction at selected temperatures. Solid lines are guides for the eyes.

experiments. One possibility for explaining these results is that the transverse lattice modulation in LaBiS₂O_{0.5}F_{0.5} is not the usual CDW state. However, as stated above, strict comparison between the experimental and calculated phonon dispersions seems to be difficult in this system at the present stage. Moreover, we do not consider the spin-orbit interaction of La and Bi ions. If one can establish the suitable calculation conditions for the calculation of phonons in this system and/or take into account other factors that we do not consider, the unstable phonons seen in the calculation may disappear. More careful investigation of the calculated phonons in this system is highly desirable.

If the transverse lattice modulation in $LaBiS_2O_{0.5}F_{0.5}$ is not the CDW state, there would be two possibilities for its origin. One is that the transverse lattice modulation in $LaBiS_2O_{0.5}F_{0.5}$ is an order-disorder-type structural transition [43-45]. As Athauda et al. reported [36,46], a local distortion due to the displacement of the S1 ions takes place within the BiS_2 plane, while the *overall* crystal structure of $LaBiS_2O_{0.5}F_{0.5}$ is well reproduced by the tetragonal one. In this case, the S1 vibrational modes corresponding to deviation from the local displacement would exist at higher energy and would not soften. Then, a correlation between the deviation from the local displacement gradually develops with decreasing temperature, finally leading to the transverse-type lattice distortion (structural transition) at $T^* \sim 260$ K. According to the energy dependence of the reported (calculated) phonon density of states for LaBiS₂O [19], the vibrations of S1 ions are dominant above ~ 10 meV. However, as our data exhibit, intensities above 10 meV are quite small (see Figs. 4 and 5), and therefore, it is difficult to determine the vibrations of S1 ions coincident with the deviation from the local displacement.

The other possibility is that the transverse lattice modulation in LaBiS₂O_{0.5}F_{0.5} is a displacive structural transition with an overdamped mode. In this case, our results are explained by considering that the line widths and the intensities of the phonon spectra are highly broadened and reduced by a strong scattering of the S1 vibrational modes. Such an overdamped mode due to the strong scattering can be seen in a system having a strong electron-phonon coupling or in a system whose displacive structural transition is close to the order-disordertype structural transition [47–50]. In the latter case, the local displacement and development of the correlation between the deviations from the local displacement coincidentally occur at the close temperatures. Therefore, a frequent fluctuation of the S1 local distortion may cause the strong scattering of the S1 vibrational modes.

The local structure distortion or the short-range correlation within the BiS₂ plane plays a key role in both proposed scenarios. In addition, all our data are measured above $T_c \sim$ 2.5 K; therefore, the relationship between the superlattice reflections and the superconductivity of this system is still unclear. Although the superlattice reflections in NdBiS₂O_{1-x}F_x were observed even below its T_c (~5 K) [22], the authors of the literature point out the possible competition between the superlattice reflections (or the CDW state) and the superconductivity regardless of their coexistence. To comprehensively understand the newly discovered transverse lattice modulation and its relationship to the superconductivity in LaBiS₂O_{0.5}F_{0.5}, further detailed studies on the local structure distortion, the lattice dynamics, and their temperature variation through T_c will be needed.

V. SUMMARY AND CONCLUSION

We performed first-principles calculations and the IXS experiments using a single crystal to investigate lattice

SL reflections of dynamics associated with the LaBiS₂O_{0.5}F_{0.5}. Our first-principles calculations of phonon dispersion and the FSs demonstrate that the phonon mode corresponding to the transverse-type lattice modulation is unstable and the phonon softening originates from the FS nesting. On the other hand, measured phonon dispersion in LaBiS₂O_{0.5}F_{0.5} along the Z-A direction shows no remarkable temperature dependence, and there are no steeply declining branches accompanied with a softening around q_{SL} . Although it is rather difficult to strictly compare the experimental phonon dispersion with the calculated one, one possibility for explaining these results is that the transverse lattice modulation in $LaBiS_2O_{0.5}F_{0.5}$ is not the usual CDW state due to the FS nesting. In stead, we discuss the two scenarios for the transverse lattice modulation in $LaBiS_2O_{0.5}F_{0.5}$, the order-disorder-type structural transition and the displacive structural transition with an overdamped mode. The local structure distortion or the short-range correlation within the BiS₂ plane is essential for both proposed scenarios.

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