

Lattice dynamics of the infinite-layer nickelate LaNiO_2

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Infinite-layer (IL) nickelates have rapidly emerged as a new class of superconductors. However, due to the technical challenges of their topotactic synthesis, they have so far been realized primarily as thin films or polycrystalline powder samples, limiting comprehensive investigations of fundamental physical properties such as the lattice dynamics. Here, we present a time-of-flight inelastic neutron scattering study on a sample composed of a large number of coaligned bulk crystals of the IL nickelate LaNiO_2 . We observe several dispersive phonon branches, which are in good agreement with lattice dynamical calculations based on density-functional perturbation theory. In addition, we compare the characteristics of selected LaNiO_2 phonon modes to those of isostructural cuprate superconductors. Our findings provide a reference point for future experimental and theoretical efforts aimed at understanding the interplay between lattice dynamics and electronic properties in IL nickelates.

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I. INTRODUCTION

The recent discovery of superconductivity in infinite-layer (IL) nickelates [1] has generated significant interest due to their structural and electronic similarities to high-temperature superconducting cuprates. In the latter, superconductivity emerges upon doping charge carriers into the CuO_2 planes, thereby suppressing the long-range antiferromagnetic order of the parent Mott-insulating state [2–5]. Nevertheless, despite decades of intensive research, consensus on the microscopic mechanism underlying unconventional superconductivity in cuprates remains elusive. Therefore, the discovery and exploration of related materials, such as IL nickelates, which might share key superconducting characteristics, offer promising opportunities to address this long-standing problem.

Striking similarities between IL nickelates of composition RNiO_2 (R : rare-earth ion) and cuprates were pointed out early in theoretical studies [6], even preceding the experimental

confirmation of superconductivity in IL nickelate thin films [1,7–12]. In particular, both material classes exhibit NiO_2 (CuO_2) planes, wherein Ni^{1+} (Cu^{2+}) ions nominally adopt a $3d^9$ electronic configuration. However, later theoretical studies predicted distinct features of the electronic structure of IL nickelates [13], including a diminished $3d$ - $2p$ hybridization between Ni and the O ligands, while at the same time rare-earth $5d$ Fermi surface pockets self-dope the Ni $3d$ bands [14–29], which explains the metallic properties of the parent RNiO_2 compounds. Signatures of this distinct electronic structure of IL nickelates have been evidenced in recent photon and electron-spectroscopic measurements [30–33].

In cuprates, the electronic structure and lattice dynamics are strongly coupled, leading to pronounced anomalies in specific phonon modes [34]. Notably, the Cu-O bond-stretching (breathing) modes exhibit anomalous softening and broadening at characteristic wave vectors, indicative of strong electron-phonon interactions [35–41]. Some of these anomalies, revealed by phonon dispersion measurements using inelastic neutron and x-ray scattering across various cuprate families, have been discussed in the context of the microscopic mechanisms driving charge density wave formation [42]. Phonons thus serve as a sensitive probe of the underlying charge correlations. Consensus holds that spin fluctuations [43,44] play a central role in the superconducting pairing mechanism in cuprates [3,5,45,46], whereas electron-phonon interactions are insufficient to account for the high superconducting transition temperatures, although phonons may still contribute to or interact with the pairing process [47–52].

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In superconducting IL nickelates, the pairing mechanism and symmetry remain under investigation. Initial spectroscopic studies on samples with potentially degraded surfaces yielded conflicting results regarding nodal versus fully gapped behavior [53–58], whereas recent ultrafast optical spectroscopy experiments suggest a weak-coupling *d*-wave pairing state [59]. Given their moderate superconducting transition temperature relative to cuprates [60,61], the role of phonons and possible lattice instabilities remains an active field of inquiry [62–66]. Theories diverge on this point, suggesting either strong electron-phonon coupling (EPC) [67–69] and phonon-driven *s*-wave gap scenarios [68,70,71], or that EPC in IL nickelates is insufficient to explain superconductivity [14,72]. In lieu thereof, spin fluctuations have been suggested as the dominant pairing mechanism [17,73], similarly to the cases of cuprates and iron-based superconductors [3].

However, in spite of numerous theoretical studies on the lattice dynamics of IL nickelates and continued debate over the role of phonons [62–68,70,72,74–78], a basic experimental characterization of their phonon spectrum is lacking. This is likely due to the demanding nature of the topotactic synthesis process, which previously limited the availability of IL nickelate samples to thin films or polycrystalline powders, preventing the acquisition of highly resolved energy- and/or momentum-dependent spectroscopic data from bulk single crystals, for instance by inelastic neutron scattering (INS). Additionally, optical spectroscopy has not been able to clearly distinguish phonons in IL nickelate films from substrate contributions [79], and no Raman-active phonon modes exist at the zone center for the *P4/mmm* structure of RNiO₂ [80,81].

In this work, we perform INS experiments on LaNiO₂ crystals, observing various branches of acoustic and optical phonons. We compare the measured phonon spectrum to lattice dynamical calculations obtained via density-functional perturbation theory (DFPT) [82] and discuss the computed dispersions in the context of characteristic phonons in cuprates, including bond stretching, buckling, and bending modes as well as charge fluctuation-coupled modes. The results establish a basis for future studies exploring the interplay between lattice dynamics, EPC, and the electronic properties of IL nickelates.

II. MATERIALS AND METHODS

Cube-shaped LaNiO₂ crystals with dimensions of approximately 1 mm³ were obtained through topotactic reduction of optical floating zone grown LaNiO₃ crystals [83,84], using CaH₂ as the reducing agent. The details of the synthesis procedure are described in Ref. [85]. More than 100 LaNiO₂ crystals with a total mass of 870 mg were coaligned on an Al grid for the INS experiment [Fig. 1(a)]. X-ray diffraction (XRD) from the surface of individual LaNiO₂ crystals [Fig. 1(b)] revealed the presence of (*H*, 0, 0)/(0, *K*, 0)- and (0, 0, *L*)-type Bragg peaks of the tetragonal *P4/mmm* space group, suggesting that the crystals contain three twin domains, as described in detail in Ref. [85]. Different intensity ratios between the Bragg peaks in the XRD patterns of different crystals [Fig. 1(b)] indicate that each crystal might exhibit a

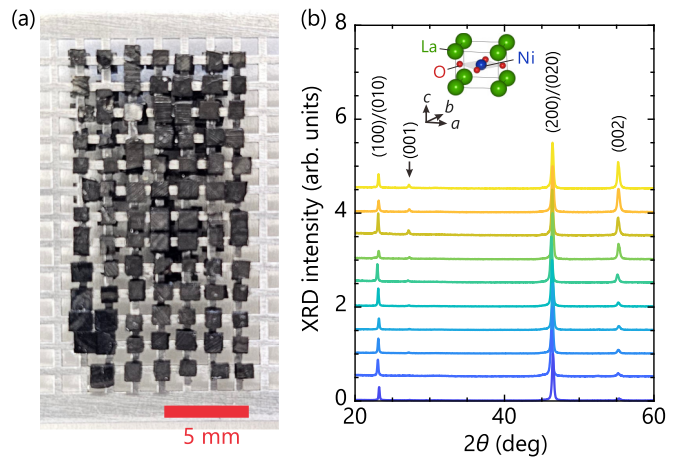


FIG. 1. (a) Sample array with coaligned LaNiO₂ crystals on two sides of an Al grid. (b) Representative XRD patterns from the surface of individual LaNiO₂ crystals, acquired with Cu *K*_α radiation at 300 K. The Bragg peaks are indexed. The inset shows the tetragonal *P4/mmm* unit cell of LaNiO₂.

distinct domain population across the probed surface region. In the INS experiment which picks up the bulk signal from the entire sample array consisting of more than 100 crystals, the varying domain populations are averaged out (see Supplemental Material [86]) and we assume an equal population of the three domains for the INS data analyses.

The INS measurements were conducted at the thermal neutron time-of-flight spectrometer PANTHER (ILL, France) [87] at 1.5 K. The energy of the incident neutron beam was $E_i = 76$ meV, yielding a Gaussian energy resolution of $\Delta E = 4.9$ meV at the elastic line. The scattering plane was chosen such that the crystallographic *ab* plane was horizontal, although we note that this reference frame applies only to one out of the three orthogonal *P4/mmm* twin domains in the sample. An Al grid sample holder without nickelate crystals was measured under the same conditions and the corresponding background signal was subtracted from all INS spectra shown in the following. Data reduction and background subtraction were performed using MANTID [88], and all data were analyzed using HORACE software [89].

To determine the ground-state crystal structures of LaNiO₂, density-functional theory [90,91] level structural relaxations were performed using VASP [92–94]. The Perdew-Burke-Ernzerhof version of the generalized gradient approximation [95] was employed, sampling the Brillouin zone (BZ) with a dense $13 \times 13 \times 15$ Monkhorst-Pack *k* mesh for a unit cell of LaNiO₂ and a $6 \times 6 \times 8$ *k* mesh for the $2 \times 2 \times 2$ supercell of LaNiO₂. Energy and force convergence criteria were set to 10^{-8} eV and 0.01 eV/Å, respectively. The experimentally determined lattice parameters of LaNiO₂ were fixed during structural relaxations while atomic positions were fully relaxed. Phonon spectra for LaNiO₂ compounds were calculated using DFPT [82] and postprocessed with the PHONOPY code [96]. The EUPHONIC software package [97,98] was employed to simulate the INS phonon intensities, using the results from the DFPT calculation as an input.

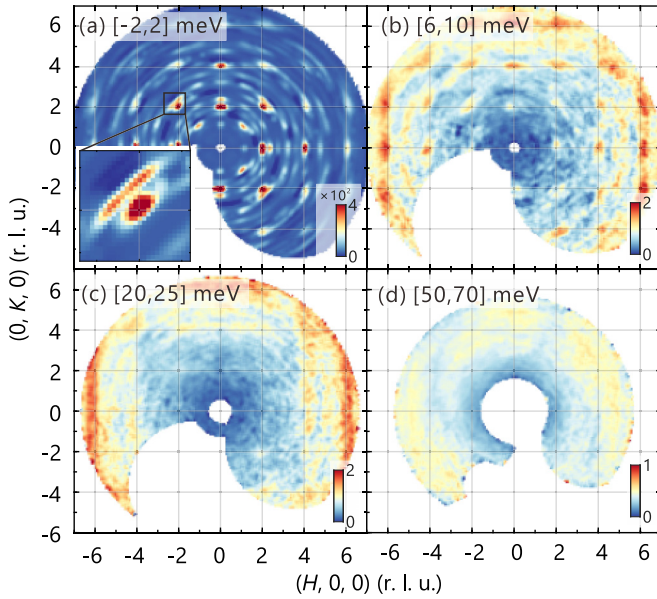


FIG. 2. (a)–(d) Constant energy slices of the INS spectra in the $(H, K, 0)$ plane for incident neutron energy $E_i = 76$ meV. The transferred energies are integrated over the following ranges: (a) $-2 \leq E \leq 2$ meV, (b) $6 \leq E \leq 10$ meV, (c) $20 \leq E \leq 25$ meV, and (d) $50 \leq E \leq 70$ meV. The integration range along the out-of-plane direction is $\pm 0.37 \text{ \AA}^{-1}$. The inset in panel (a) highlights two satellite peaks from $P4/mmm$ twin domains around the $(-2, 2, 0)$ Bragg peak.

III. RESULTS

Figures 2(a)–2(d) display neutron scattering intensity maps in the $(H, K, 0)$ plane acquired with $E_i = 76$ meV at the PANTHER spectrometer. The H, K, L indexing refers to the LaNiO_2 twin domain with the crystallographic ab plane lying in the scattering plane, denoted as *domain 1* in the following. In the quasielastic scattering map in Fig. 2(a) (energy integration range: $-2 \leq E \leq 2$ meV), Bragg peaks emerge at integer H and K positions, exhibiting a rather smeared out intensity distribution. The peaks are particularly intense for even H and K values, which is consistent with the structure factor of LaNiO_2 in the $P4/mmm$ space group. In addition, satellite peaks occur in proximity to the Bragg peaks at slightly deviating H and K values [see inset in Fig. 2(a)]. These peaks originate from the other two twin domains of the tetragonal $P4/mmm$ space group of LaNiO_2 , denoted as *domain 2* and *domain 3* in the following. In a previous XRD study on individual LaNiO_2 crystals, similarly broad Bragg peak intensity profiles and satellite peaks were observed in XRD maps of the $(H, K, 0)$ plane [83], suggesting that the total mosaicity of the sample array used for the present INS experiment is comparable to that of individual crystals.

In the inelastic scattering map in Fig. 2(b) with energy range $6 \leq E \leq 10$ meV, pronounced accumulations of spectral weight occur around even H and K values, indicating the presence of characteristic low-energy excitations. The intensity of the spectral weight accumulations increases for larger $\mathbf{Q}$, which is opposite to the trend in the quasielastic scattering in Fig. 2(a). This intensity increase for larger $\mathbf{Q}$ suggests that the excitations are likely phonons, due to the

normal phonon polarization factor. For energy transfers above 20 meV [Figs. 2(c) and 2(d)], the spectral weight accumulations become less localized and their intensity fades out.

To further investigate the excitations revealed in Figs. 2(b)–2(d), we next inspect an INS intensity map along a high-symmetry path in the BZ, generated from folded data around the (060) and (600) Bragg peaks. Figures 3(a) and 3(b) display the folded quasielastic and inelastic scattering maps in the $(H, K, 0)$ plane, respectively, and Fig. 3(c) shows a schematic of the high-symmetry path within the $P4/mmm$ unit cell. In the corresponding INS map [Fig. 3(d)], we find that inelastic, dispersive spectral weight emanates from the Γ point, while flat branches extend across wide paths in the BZ around 15 and 30 meV, connecting the X and M point as well as the R and A point. Additionally, a broad distribution of spectral weight occurs below 30 meV in the region between Γ and Z .

To corroborate that the observed spectral weight in Fig. 3(d) originates from phonons, we compute the phonon dispersion in LaNiO_2 using DFPT. As an input for the DFPT calculation, we use the refined lattice parameters of the $P4/mmm$ unit cell from the INS experiment (see Supplemental Material [86]). Furthermore, since the investigated sample contains three twin domains, we project the computed phonon dispersions of domains 2 and 3 onto the Γ - X - M - Γ - Z - R - A - Z path of domain 1. Notably, the superimposed DFPT dispersions of acoustic and optical phonon branches closely match the INS spectral weight distribution in Fig. 3(d), including the steeply dispersing bands emanating from Γ and the relatively flat bands between X and M as well as R and A . However, while the experimentally observed spectral weight is sharply confined below ≈ 38 meV, the DFPT calculations predict several phonon branches extending up to ≈ 68 meV.

For a closer comparison between theory and experiment, we simulate the INS phonon intensity of LaNiO_2 using the EUPHONIC software package [97,98], with DFPT-derived eigenenergies and eigenvectors (see Fig. 4 below) of the phonons as input. Figure 3(e) displays the resulting simulated intensity map, averaged over all three domains. In addition, adequate Gaussian broadenings were applied in both momentum and energy transfer directions in the map in Fig. 3(e) (for details see Supplemental Material [86]). Notably, the simulation not only reproduces the absence of significant phonon intensity above ≈ 38 meV, but also qualitatively captures key features from Fig. 3(d), such as the spectral weight accumulation around the Γ - Z region and the intense flat bands between X and M as well as R and A .

In general, the diminishing INS intensity observed in LaNiO_2 above ≈ 38 meV can be attributed to several factors, including that the one-phonon scattering cross section decreases with increasing phonon energy, scaling approximately as $1/\omega$, which naturally reduces intensity at higher energies. In addition, the high-energy phonons in LaNiO_2 predominantly involve oxygen bending and stretching modes with out-of-phase displacements between some of the neighboring oxygen atoms, reducing the net scattering amplitude.

IV. DISCUSSION

The close agreement between the measured phonon signal and the DFPT results for modes below ≈ 38 meV suggests

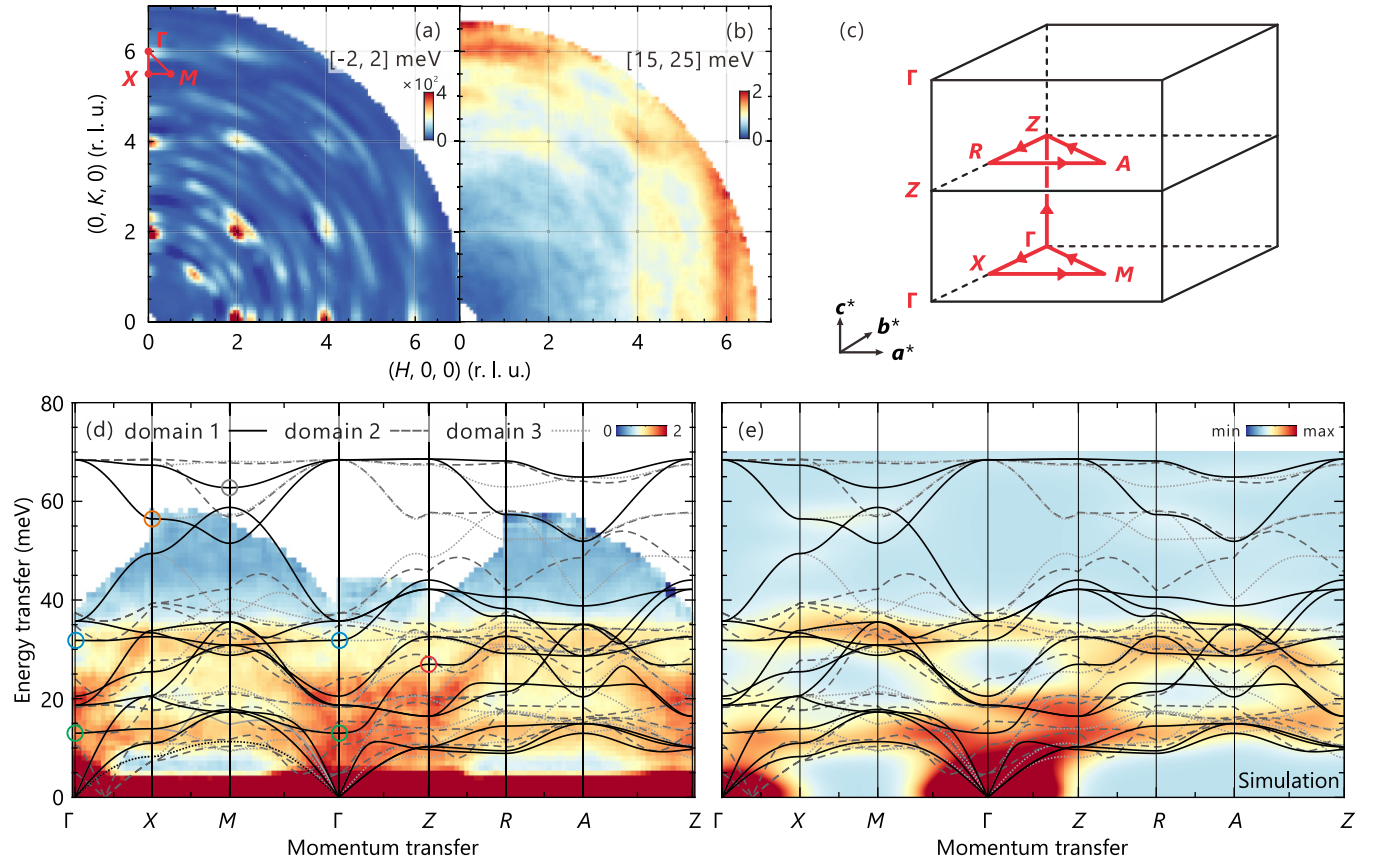


FIG. 3. (a), (b) Constant energy slices of folded INS spectra in the $(H, K, 0)$ plane for incident energy $E_i = 76$ meV. The transferred energies are integrated over the following ranges: (a) $-2 \leq E \leq 2$ meV and (b) $15 \leq E \leq 25$ meV. A path along high-symmetry points (Γ -X-M- Γ) is illustrated in red color around the (060) Bragg reflection in panel (a). (c) Schematic of a three-dimensional path moving along the high-symmetry points Γ -X-M- Γ -Z-R-A-Z according to the tetragonal $P4/mmm$ unit cell of LaNiO_2 . (d) INS map along a high-symmetry path from folded data around the (060) and (600) Bragg peaks, acquired with $E_i = 76$ meV. The integration range along the two orthogonal directions relative to the path is $\pm 0.2 \text{ \AA}^{-1}$. The DFPT computed phonon dispersions for the three twin domains of LaNiO_2 are superimposed as solid (domain 1), dashed (domain 2), and dotted lines (domain 3). The colored circles on the dispersion curves of domain 1 indicate specific phonon modes discussed in the text. (e) Phonon intensities calculated with the EUPHONIC software package, using the DFPT phonons as input. The intensities are averaged over the three domains, while the indexing of the high-symmetry path refers to domain 1. In addition, Gaussian broadening is applied along both the momentum ($\Delta Q = 0.92 \text{ \AA}^{-1}$) and energy ($\Delta E = 4.9$ meV) transfer directions. Details about the domain averaging and broadening are given in the Supplemental Material [86].

that this theoretical approach quite reliably captures the essential lattice dynamics of LaNiO_2 . Hence, we next discuss selected DFPT calculated phonon modes in detail, also drawing comparisons to related modes in cuprates, which were intensively investigated by INS [35–41].

A comprehensive overview of the phonon modes in LaNiO_2 along with the DFPT computed energies is presented in Fig. 4. At the Γ point, the lowest-energy optical phonon exhibits a computed energy of 13.0 meV [green circle in Fig. 3(d)], involving an antiphase motion between La and Ni ions along the c -axis direction [Fig. 4(a)]. The dispersion of the mode between Γ and X is nearly flat, which is reminiscent of the analogous mode in the isostructural IL cuprate SrCuO_2 [99]. A second notable Γ -point mode [blue circle in Fig. 3(d)] at 31.8 meV involves in-phase movements of La and Ni against the O atoms [Fig. 4(a)]. This mode also displays minimal dispersion towards X. In cuprates, *ab initio* rigid-ion model calculations suggest that such modes involving axial displacements of the O sublattice against

the cation sublattices can split into longitudinal optical and transverse optical branches [99] and are associated with ferroelectric instabilities. However, this splitting is suppressed under metallic screening conditions [99], consistent with the metallic ground state and absence of ferroelectric behavior in LaNiO_2 [85].

At the X point, the 56.5-meV phonon [orange circle in Fig. 3(d)] corresponds to the oxygen half-breathing mode (HBM), characterized by the in-plane motion of the O ions along the Ni-O bond direction such that alternating oxygen atoms are displaced towards and away from a central Ni [Fig. 4(b)]. The analogous HBM in the IL cuprate SrCuO_2 was theoretically described in Ref. [99] and experimentally observed by INS in related cuprates at comparable energies [36], for instance, at 58.5 meV in $\text{HgBa}_2\text{CuO}_{4+\delta}$ [38]. Interestingly, this longitudinal zone boundary mode shows strong renormalization effects in doped cuprates below the superconducting transition, underlining the relevance of the HBM also for IL nickelates and warranting

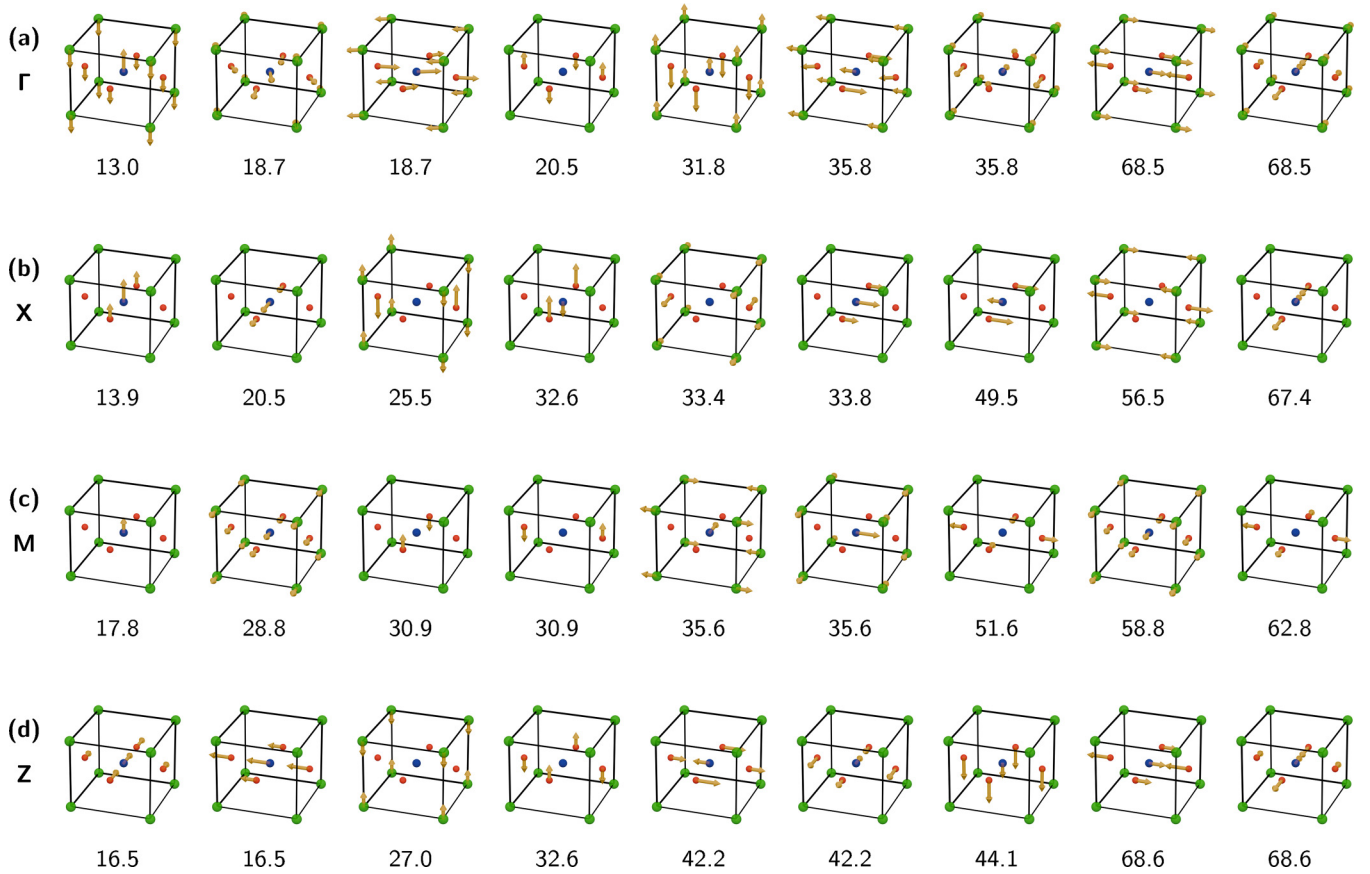


FIG. 4. (a) Atomic displacement patterns of selected phonons of LaNiO_2 at the Γ point together with the computed phonon energies in units of meV. La atoms are shown in green, Ni in blue, and oxygen in red. The yellow arrows indicate the directions and amplitudes of the atomic vibrations. For clarity, the La, Ni, and O atoms are displayed with reduced atomic radii. (b)–(d) Displacement patterns of phonons at the X, M, and Z points, respectively.

future experimental studies with techniques that can resolve the mode.

At the M point, the highest-energy phonon mode, located at 62.8 meV [gray circle in Fig. 3(d)], corresponds to the full-breathing mode (FBM), in which all oxygen ions move uniformly in phase toward or away from the central Ni ion [Fig. 4(c)]. In cuprates, oxygen breathing distortions, such as the HBM and FBM, are known to be selectively sensitive to the on-site Coulomb repulsion U_d of the localized Cu $3d$ orbitals [100–102], with an increased U_d suppressing charge fluctuations at the Cu site, resulting in a hardening of the breathing mode. In contrast, the smaller U_d on Ni in IL nickelates generally leads to softer breathing modes compared to their cuprate counterparts. This trend was recently examined in LaNiO_2 by *ab initio* many-body methods [77], suggesting that the energy of oxygen breathing modes may serve as an indirect but sensitive probe of electronic correlation strength in this material class.

Notably, the INS map in Fig. 3(d) shows no additional spectral weight around the M point beyond that attributable to phonons. In particular, we find no indication of spin excitations at the M point, also not in an analysis focused on small $\mathbf{Q}$ where the magnetic signal is expected to be strongest (see Supplemental Material [86]). This absence is noteworthy given that the M point corresponds to the antiferromagnetic zone center in square-lattice Heisenberg antiferromagnets,

where a pronounced low-energy magnetic response in this region is well established for cuprates [103]. Moreover, resonant inelastic x-ray scattering experiments on IL nickelate thin films [104–106] as well as on LaNiO_2 crystals from the same synthesis batch [85] have revealed spin excitations consistent with paramagnons arising from $S = 1/2$ square-lattice Heisenberg-type correlations. This can be explained by our estimate of the expected INS signal strength for spin excitations in IL nickelates (see Supplemental Material [86]), which suggests that a significantly larger sample mass is required to resolve magnetic features in the present experiment.

At the Z point, the 27.0-meV phonon [red circle in Fig. 3(d)] involves an axial breathing motion of the La ion against the NiO_2 planes [Fig. 4(d)]. In IL cuprates, the analogous mode has been reported to couple strongly to charge fluctuations [99], typically manifesting as phonon linewidth broadening due to EPC, an effect that has been extensively studied in various cuprate compounds, offering important insights into the interplay between lattice dynamics and electronic correlations [107]. Dynamical interplane charge transfer due to the axial breathing mode is expected to be particularly enhanced in compounds with a short c -axis lattice parameter [99], such as the recently synthesized Sm-based IL nickelates that might exhibit an enhanced T_c [108,109]. In Fig. 3(a), in principle, the broad spectral weight distribution observed between Γ and Z could result from EPC-induced

broadenings, consistent with the predicted presence of strong EPC in IL nickelates [67,68,70,78] and the coupling of certain modes with appropriate symmetry along the c direction to charge fluctuations via EPC [99]. However, the limited resolution and statistical quality of our current data preclude an unambiguous assessment of this effect in Fig. 3(d). Future high-resolution INS studies on LaNiO_2 crystals with higher crystalline quality and a possibly monodomain character will be necessary to clarify the effect of EPC on certain modes and its general role in IL nickelates.

V. CONCLUSION

In summary, we have investigated the lattice dynamics of LaNiO_2 on a sample of coaligned bulk crystals. Several branches of acoustic and optical phonons were observed below ≈ 38 meV, in good agreement with lattice dynamical calculations based on DFPT. Simulated INS intensity maps, incorporating DFPT mode-resolved eigenvectors and domain averaging, reproduced the main features of the experimental spectra and account for the lack of observable high-energy phonons that are dominated by oxygen displacements.

Based on our DFPT results, we have identified and discussed several characteristic phonon modes, including the HBM at the X point and the FBM at the M point, which are of particular relevance in the context of related cuprate superconductors. Furthermore, our computational results may also assist in the assignment of infrared-active phonons as well as phonon-induced features observed in other spectroscopic probes such as angle-resolved photoemission spectroscopy [32,33]. While direct signatures of spin wave excitations and EPC-induced phonon broadening could not be resolved in the

present data, such effects may become observable in future high-resolution INS studies on higher-quality and larger-mass LaNiO_2 crystals. Overall, our results establish an experimental foundation for understanding the lattice dynamics of IL nickelates and lay the groundwork for future investigations addressing electron-phonon interactions, structural instabilities, and their possible relevance to superconductivity in this material class.

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DATA AVAILABILITY

The data that support the findings of this article are openly available [110].

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