

Optical properties of MoOCl₂: Anisotropic plasma frequencies, effective masses, and interband excitations

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MoOCl₂ is a metallic, layered van der Waals material with a strong in-plane structural anisotropy. The reflectivity of a MoOCl₂ single crystal has been determined in a wide spectral range from the infrared to the visible regime. This reflectivity is extremely anisotropic, reflecting the anisotropic crystal structure and electronic properties of MoOCl₂. Using a Drude–Lorentz fit, we extracted the dielectric function quantitatively for the two in-plane directions of MoOCl₂, and we determined the anisotropic optical effective mass of the conduction electrons. Our data additionally demonstrate the presence of interband excitations in the measured spectral range.

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I. INTRODUCTION

Layered van der Waals (vdW) crystals have been the subject of a large number of scientific investigations because of their rich electronic properties and potential applications [1–7]. Initiated by the isolation of graphene, a variety of materials emerged, and these harbor interesting and tunable properties, as, for instance, thickness-dependent band gaps [8,9], strong excitonic effects [10,11], unconventional surface superconductivity [12,13], topological electronic phases [14,15] or intrinsic two-dimensional magnetic states [16,17]. One of their key features is their intrinsic uniaxial anisotropy, resulting from the strongly anisotropic bonds in the crystals. More recently, some further members of the material class that exhibit an in-plane biaxial anisotropy have moved into the focus of research. Amongst the latter, transition-metal oxyhalides with the general composition MOX₂ (*M* = transition metal, *X* = halogen) recently emerged as a quite promising

family of vdW crystals, since they demonstrate, e.g., large in-plane optical anisotropy and a quasi-one-dimensional (1D) Fermi surface [18–22]. In addition, the highly anisotropic MoOCl₂ and RuOCl₂ are predicted to be promising candidates for supporting broadband hyperbolic plasmon polaritons in the visible to near-infrared range [20,23–29].

The vdW oxyhalides share a characteristic structural motif of metal-oxygen chains coordinated by halide atoms. In the case of MoOCl₂, the substantial anisotropic electronic properties have been ascribed to an orbital-selective Peierls phase, which causes the formation of quasi-1D Mo–Mo dimerized chains within the vdW layers [19]. The formation of these dimers results in the localization of conduction electrons along one crystal direction and a quasi-1D electronic structure [18,21].

In this contribution, we present polarization-dependent measurements of the reflectivity of MoOCl₂ crystals in an energy range from the infrared regime up to the visible. Our data confirm previous reports and demonstrate the very large in-plane optical anisotropy of MoOCl₂. Furthermore, we have applied the Drude–Lorentz model to describe the measured reflectivities, which allowed us to identify the anisotropic plasma frequencies and optical effective masses quantitatively, as well as the energy window in which MoOCl₂

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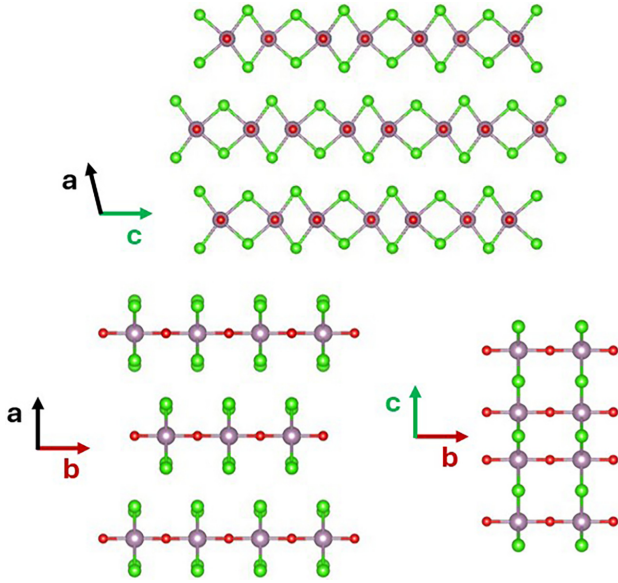


FIG. 1. Illustration of the MoOCl_2 crystal structure. The atoms are drawn in gray (Mo), red (O), and green (Cl). In the crystal $\mathbf{c}$ direction, the $\text{Mo-Cl}_2\text{-Mo}$ chains are dimerized (see text), which is clearly seen by the varying distances in the Figure.

is expected to support hyperbolic plasmon polaritons. Our analysis additionally indicates the contributions of interband excitations in the measured energy range.

II. EXPERIMENTAL AND DATA ANALYSIS

MoOCl_2 is a layered vdW material belonging to the subgroup of oxychlorides, whose crystal structure is characterized by a monoclinic lattice (space group $C2/m$) [30,31]. The structure of a single layer of the MoOCl_2 crystal consists of a central plane made of Mo–O chains (extending in the $[010]$ direction). The in-plane lattice takes a rectangular structure, with orthogonal unit-cell vectors $\mathbf{b}$ and $\mathbf{c}$ with sizes 3.75 Å and 6.52 Å, respectively. In the bulk structure, the monolayers are stacked and shifted such that the $[100]$ direction is not parallel to the layer normal, resulting in a unit vector $\mathbf{a}$ of 12.72 Å and a monoclinic angle β of 104.86° [31], see Fig. 1.

MoOCl_2 single crystals were successfully grown using the chemical vapor transport method. A quartz ampoule (~20 cm in length) was charged with MoCl_3 (99.5% purity) and MoO_3 (99.97% purity) in a molar ratio of 2:1. The ampoule was repeatedly purged with argon and evacuated before being flame-sealed under mild vacuum (~1 Pa). The sealed ampoule was placed in a horizontal two-zone furnace and heated to source and sink temperatures of 450 °C and 350 °C, respectively, with controlled ramp rates of 0.32 °C/min for the source zone and 0.24 °C/min for the sink zone. This temperature gradient was maintained for one week, after which the furnace was slowly cooled down to room temperature for two days. Bronze-colored, needle-like MoOCl_2 single crystals with widths on the millimeter scale and lengths up to the centimeter scale were obtained at the sink end of the ampoule. Energy-dispersive X-ray spectroscopy (EDX) was performed at 15 spots of the crystal used in this study for elemental analy-

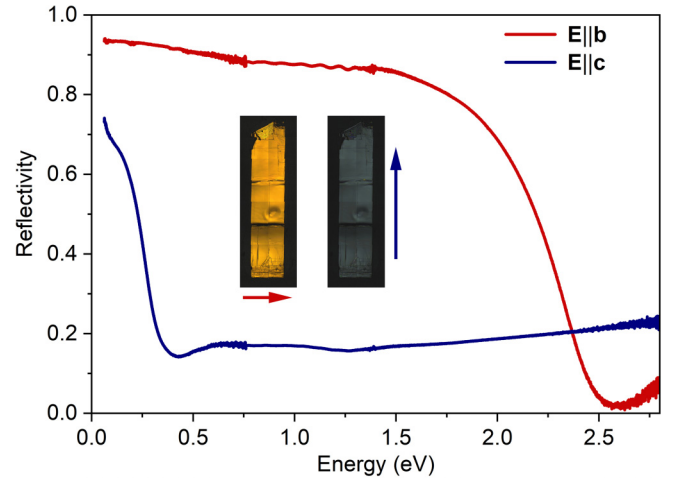


FIG. 2. Measured reflectivity of a MoOCl_2 single crystal (solid lines) with the light polarization vector oriented along the $\mathbf{b}$ and $\mathbf{c}$ crystal axes ($\mathbf{E}||\mathbf{b}$ and $\mathbf{E}||\mathbf{c}$). In addition, we show the visual appearance of the single crystal for the two polarization directions. The size of the two insets is 5 × 1 mm.

sis. This validated the expected composition (MoOCl_2) within the measurement errors. Electron diffraction performed in a transmission electron microscope confirmed the monoclinic crystal structure [30,31] (see Appendix).

The reflectivity in the $\mathbf{bc}$ plane of MoOCl_2 was determined at room temperature in an energy range from 50 meV to 2.5 eV using a Bruker Vertex spectrometer equipped with the Hyperion 2000 microscope extension. For these measurements, a fresh crystal surface was prepared by peeling a thin flake of the crystal using blue tape. The crystals were placed under the microscope and oriented to achieve the optimal reflection geometry. To cover the spectral range from the infrared to the visible, different light sources (glow bar, halogen lamp) and detectors (HgCdTe, InGaAs, and Si diode) were used. Furthermore, three different polarizers were employed to ensure optimal light polarization across the entire spectral range. Gold and silver mirrors were used as reference.

We analyzed the polarization-dependent integrated reflectivity in the visible to establish the orientation of the crystal $\mathbf{b}$ and $\mathbf{c}$ axes in our measurement setup. In Fig. 2, we show the maximal optical anisotropy of our crystal and the corresponding light polarization. Note that the two polarization directions follow the short and long axes of the single crystal, in good agreement with previous results [21].

We modeled our data using the well-known Drude–Lorentz model [32], in which the dielectric function is given by

$$\epsilon(\omega) = \epsilon_\infty - \frac{\omega_D^2}{\omega^2 + i\gamma_D\omega} + \sum_j \frac{\omega_{pj}^2}{\omega_j^2 - \omega^2 - i\gamma_j\omega}, \quad (1)$$

$$\omega_D^2 = \frac{ne^2}{\epsilon_0 m^*}. \quad (2)$$

Here, ω_D and γ_D represent the plasma frequency and damping (scattering rate) of the conduction electrons, respectively; ω_{pj} , ω_j , and γ_j represent the oscillator strength, energy position, and spectral width of the Lorentz oscillators, respectively; and

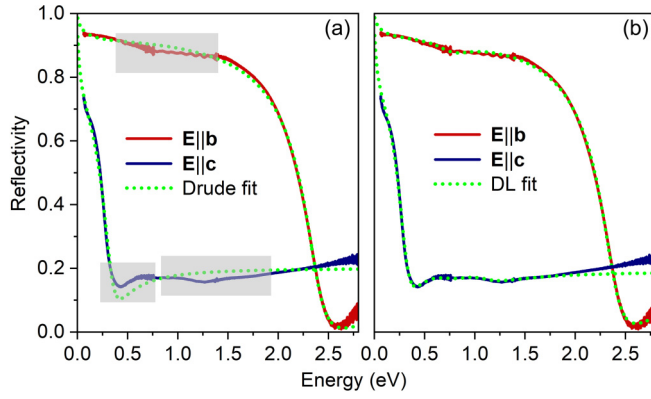


FIG. 3. Measured reflectivity of a MoOCl₂ single crystal (solid lines) with the light polarization vector oriented along the **b** and **c** crystal axes ($\mathbf{E} \parallel \mathbf{b}$ and $\mathbf{E} \parallel \mathbf{c}$). (a) In the left panel, we additionally show the result of a simple Drude fit to the measured curves. Regions where this fit does not describe the measured curves well are highlighted in gray. (b) The right panel shows the result of our fit using a Drude-Lorentz (DL) approach as described in the text.

ϵ_∞ represents the dielectric background (screening contribution) from energetically higher-lying excitations. The Lorentz terms effectively describe the contribution of interband excitations to the optical properties. The Drude (conduction electron) plasma frequency ω_D is related to the conduction electron density n and the optical effective mass m^* , e is the elementary charge, and ϵ_0 the vacuum permittivity.

III. RESULTS AND DISCUSSION

In Fig. 2, we show the reflectivity spectra of MoOCl₂ measured with light polarization along the **b** and **c** crystal axes ($\mathbf{E} \parallel \mathbf{b}$ and $\mathbf{E} \parallel \mathbf{c}$), respectively. This Figure demonstrates the very large in-plane optical anisotropy of MoOCl₂, and our data are in very good agreement with previous reports [20,21,24]. Both curves in Fig. 2 are characterized by a relatively sharp reflectivity (plasma) edge at about 2.25 eV and 0.25 eV. Such a plasma edge indicates a metallic ground state of the material, but with very anisotropic in-plane conductivity. Moreover, both curves show a minimum in reflectivity right above the plasma edge, which is a signature of contributions from higher-lying electronic excitations.

To obtain a more quantitative insight into the optical properties of MoOCl₂, we have fitted both reflectivity curves using the Drude-Lorentz approach described above. In agreement with the visible inspection of Fig. 2, both reflectivity curves can be described reasonably well by a simple Drude contribution, representing the response of the conduction electrons, and a dielectric background. This is outlined in the left panel of Fig. 3, where we depict the result of such a Drude fit for both directions. Figure 3 (left panel) additionally reveals small but visible deviations between the measured curves and the fitting results. These are highlighted by a gray background. These deviations indicate the presence of further electronic excitations at the corresponding energies, which must arise from interband excitations in MoOCl₂.

TABLE I. Parameters of a Drude-Lorentz fit to the measured reflectivities of MoOCl₂ with light polarizations $\mathbf{E} \parallel \mathbf{b}$ and $\mathbf{E} \parallel \mathbf{c}$. See Fig. 3 for the fitted curves. We estimate the uncertainty in these parameters to be about 2.5%, which mainly results from the potential misalignment (a few degrees) of the sample or the reference crystals in our measurements. Additionally, the optical effective mass m^* is given in units of the free electron mass m_0 (see text).

Parameter	$\mathbf{E} \parallel \mathbf{b}$ (eV)	$\mathbf{E} \parallel \mathbf{c}$ (eV)
ω_D	6.56	0.93
γ_D	0.27	0.17
ω_{p1}	1.77	0.66
ω_1	0.82	0.7
γ_1	0.44	0.55
ω_{p2}		0.6
ω_2		1.1
γ_2		0.45
ϵ_∞	8.1	6.53
m^*	0.4	5.1

To account for the entire form of the reflectivities in the fit, the inclusion of Lorentz terms, which model the presence of interband excitations, is necessary. In more detail, for $\mathbf{E} \parallel \mathbf{b}$ the small dip in the reflectivity around 0.8 eV indicates an interband contribution at this energy, whereas an exact fit of the reflectivity for $\mathbf{E} \parallel \mathbf{c}$ requires the inclusion of two Lorentz terms located at about 0.7 eV and 1.1 eV. The right panel of Fig. 3 demonstrates that the inclusion of such Lorentz terms results in an almost perfect description of the measured reflectivity data. The individual parameters arising from these fits are summarized in Table I.

In addition, we have calculated the expectation value for ω_D for the case of a free electron gas without mass renormalization ($m^* = m_0$, where m_0 is the free electron mass) [see Eq. (2)]. We emphasize that this expectation value for ω_D is also anisotropic or direction-dependent as a consequence of the orbital-selective Peierls ground state [19], and the strongly anisotropic electronic structure of MoOCl₂ [18,21]. Formally, Mo in MoOCl₂ has a $4d^2$ configuration. The formation of the orbital-selective Peierls ground state localizes one of these d electrons in the resulting bonding orbital of the dimers [19]. Thus, only one electron in the Mo $4d$ levels is left for the conduction bands in this material. Furthermore, the unit cell of MoOCl₂ contains four Mo atoms, which results in a conduction electron density n of four electrons per unit cell volume. Indeed, four bands with sizable dispersion cross the Fermi level parallel to the **b** direction [18,21], confirming this conduction electron density. This density now gives $\omega_D^b(m^* = m_0)$ to be about 4.2 eV. Along the **c** direction, however, the band structure calculations predict four flat bands, resulting from the Peierls distortion, and only one of them crosses the Fermi level [18,21]. The estimation of $\omega_D^c(m^* = m_0)$ was therefore performed assuming a conduction electron density of only one electron per unit cell, and we obtained about 2.1 eV. Comparing these values with those obtained from our fit to the reflectivity data (see Table I) allows the determination of the optical effective mass m^* of the conduction electrons in the **bc** plane of MoOCl₂. These results are summarized in Table I (in units of the free electron mass m_0).

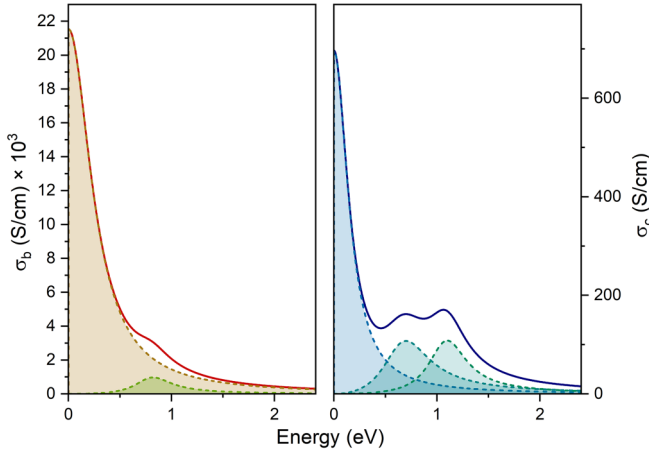


FIG. 4. Optical conductivity $\sigma = \omega\epsilon_0\epsilon_2$ for $\mathbf{E}||\mathbf{b}$ and $\mathbf{E}||\mathbf{c}$, respectively. The curves have been calculated using the parameters listed in Table I.

Looking at our results in Table I makes clear that the very large optical anisotropy of MoOCl_2 is predominantly the result of a highly anisotropic conduction electron effective mass m^* , i.e. a strongly anisotropic mobility of the conduction electrons. This is in very good agreement with the calculated orbital-selective Peierls ground state of this material [19], which essentially results in a dimerization of the MoCl_2 chains along the $\mathbf{c}$ axis and is connected to localized dimer states, radically reducing the mobility of the corresponding electrons. Other Mo $4d$ orbitals remain delocalized, i.e., the electrons are itinerant. The highly anisotropic bonding geometry in MoOCl_2 also renders the band structure highly anisotropic. As mentioned above, density-functional theory calculations provided essentially four flat bands along the $\mathbf{c}$ direction, with only one of them crossing the Fermi level [18,21]. Along $\mathbf{b}$, in contrast, all four bands cross the Fermi level with a sizable dispersion and a total conduction band width of about 3 eV [18,21]. As a consequence, the Fermi surface consists of three parallel one-dimensional sheets and a small anisotropic electron pocket [18]. Angle-resolved photoemission data qualitatively confirm this picture [21].

As mentioned above, our reflectivity data agree well with previously published data [20,21,24]. They, however, allow the additional identification of interband excitations in both polarization directions in the energy region around 1 eV (see Table I). Given the anisotropic band structure of MoOCl_2 , it is not surprising that our reflectivity data indicate the presence of interband excitations in the studied energy range. In both directions, the band structure consists of four parallel bands with vastly different dispersion. Moreover, within an energy window of about 1 eV there is a further unoccupied flat band [18]. Therefore, interband excitations on the order of 1 eV can be expected from these calculations. In Fig. 4, we show the contribution of these excitations to the optical conductivity, $\sigma = \omega\epsilon_0\epsilon_2$, in addition to the conduction electrons.

Figure 4 demonstrates that the optical properties of MoOCl_2 for $\mathbf{E}||\mathbf{b}$ are dominated by a large free-electron (Drude) contribution; the material is thus a good metal in this direction. For $\mathbf{E}||\mathbf{c}$, however, the free electron contribution is much smaller while the relative contribution of the interband

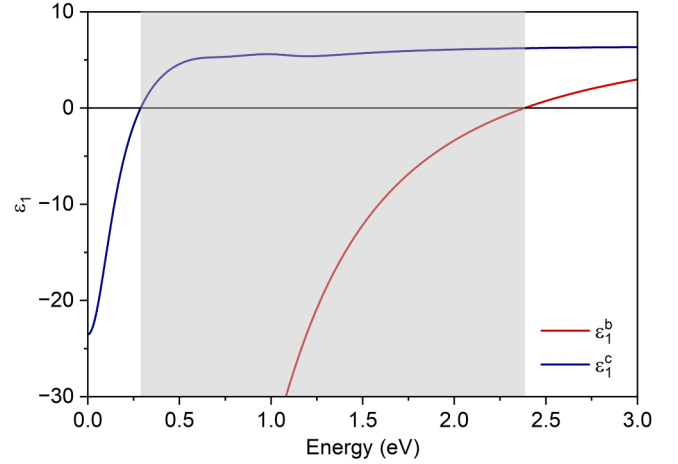


FIG. 5. Real part of the dielectric function $\epsilon_1^{b,c}$ for $\mathbf{E}||\mathbf{b}$ and $\mathbf{E}||\mathbf{c}$, respectively. The curves have been calculated using the parameters listed in Table I. The energy window where $\epsilon_1^b < 0$ and $\epsilon_1^c > 0$ is highlighted in gray.

excitations is much larger, and we expect the latter to have a much stronger impact on the properties in this direction. Recently, interband contributions to the dielectric function have been calculated for MoOCl_2 monolayers [33]. Given the rather weak interlayer interactions in vdW crystals, we expect such calculations to also provide insight into the bulk structures. Indeed, these calculations predict interband excitations at about 0.9 eV for $\mathbf{E}||\mathbf{b}$ and at about 0.75 eV and 1 eV for $\mathbf{E}||\mathbf{c}$, which is in very good agreement with our results.

Finally, our data also allow us to determine ϵ_1 , the real part of the dielectric function of MoOCl_2 for $\mathbf{E}||\mathbf{b}$ and $\mathbf{E}||\mathbf{c}$, as shown in Fig. 5. The large anisotropy of the measured reflectivities is represented by the very different zero-crossing energies of the two curves in Fig. 5. In general, a material with components ϵ_1^b and ϵ_1^c that have opposite signs ($\epsilon_1^b < 0$ and $\epsilon_1^c > 0$ in our case) can support plasmon polaritons with hyperbolic wavefronts. MoOCl_2 is characterized by a rather broad hyperbolic regime ranging from about 0.29 eV to 2.38 eV, in good agreement with previous works [20,21,24–26].

IV. SUMMARY

We have experimentally determined the anisotropic reflectivity of MoOCl_2 in the $\mathbf{bc}$ crystal plane. These data have been modeled using a Drude–Lorentz approach, which provided insight into the electronic/optical properties of this material. The plasma frequency and the conduction-electron effective mass are highly anisotropic: MoOCl_2 is a good metal along the $\mathbf{b}$ direction, but it is poorly conducting along the $\mathbf{c}$ direction. Our analysis demonstrated the presence of additional interband excitations, which reflect the particular band structure of MoOCl_2 . Finally, our data confirm that MoOCl_2 harbors a rather large hyperbolic regime where the in-plane components of the real part of the dielectric function have opposite signs.

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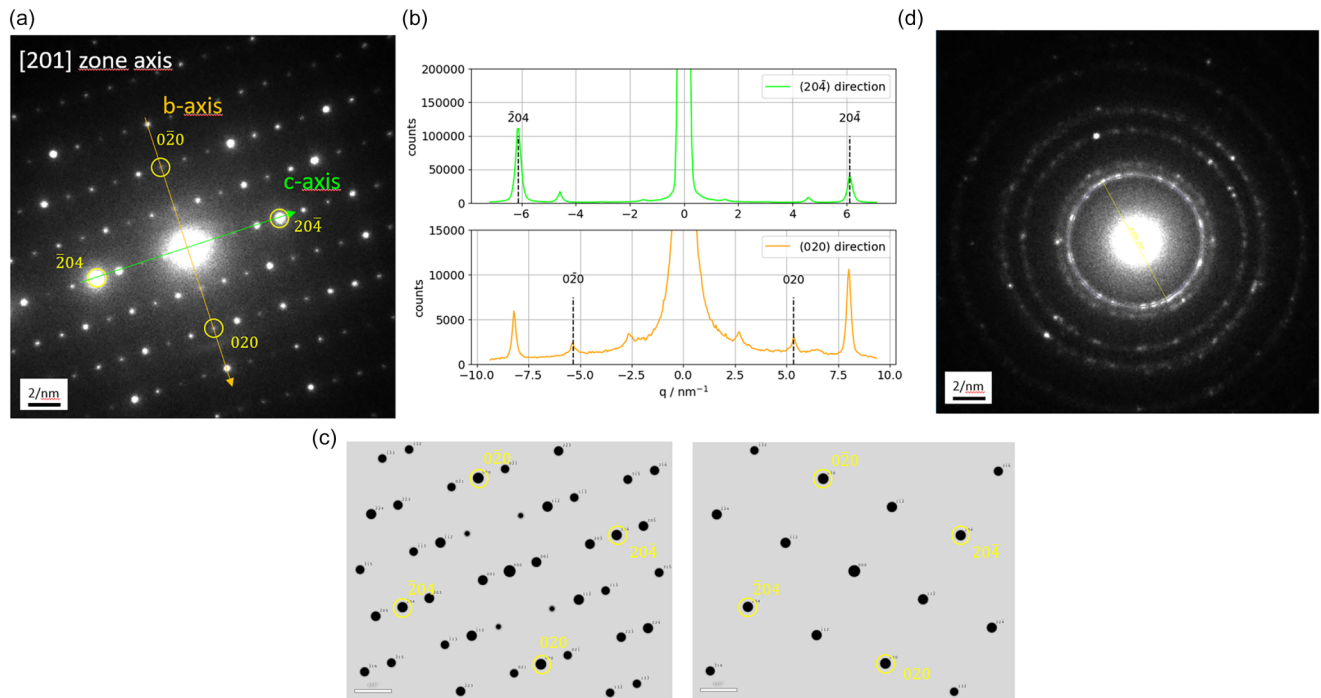


FIG. 6. (a) Electron diffraction pattern in [201] zone orientation (=layer normal). (b) intensity profiles along $(20\bar{4})$ and (020) reciprocal directions in green and orange, respectively. Peak positions expected from the structure model are indicated by dashed vertical lines. (c) Kinematic diffraction pattern simulated for a monolayer (left) and a thicker crystal (right). (d) Reference diffraction pattern of Au nanoparticles used for calibration.

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DATA AVAILABILITY

The data that support the findings of this article are not publicly available because of legal restrictions preventing unrestricted public distribution. The data are available from the authors upon reasonable request.

APPENDIX

The results of the crystal characterization using electron diffraction are shown in Fig. 6.

A thin film was prepared by mechanically exfoliating our crystal. The thin film was transferred to a transmission electron microscopy grid and characterized in a Hitachi HF3300S equipped with a QuantumDetectors Merlin4R direct electron detector. The electron microscope was operated at an accelerating voltage of 300 kV and a camera length of 1.6 m. A gold nanoparticle sample was used to calibrate the diffraction plane. The data recording and evaluation were conducted with CEOS Panda Rhei and Python. Kinematical diffraction patterns were simulated with SingleCrystal.

Figure 6(a) shows a diffraction pattern of the MoOCl₂ film oriented along the [201] zone axis, which corresponds to the layer normal direction. In the monoclinic crystal system, the reciprocal direction (020) corresponds to the **b** axis and $(20\bar{4})$ corresponds to the **c** axis. The measured reflection positions are in very good agreement with the expected values derived from the structure model [31], as shown by the corresponding line profiles in Fig. 6(b). Note that some intermediate reflections occur because of the thin sample, as illustrated by the kinematic diffraction pattern [thin foil effect, Fig. 6(c)].

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