

Anomalous bending and transmission at the Bragg condition by crystal stacking fault

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We observed an anomalous bending and transmission at the Bragg condition by crystal stacking fault. Two macroscopic and sharp deflections were observed in the proximity of the interface of stacking faults inside a diamond crystal due to the x-ray translation effect. Anomalous high transmissivity through the crystal was observed due to the x-ray translation toward the interface and due to some possible topological effect. The Berry phase for translated x-rays enables us to identify the type of stacking faults existing in the crystal by the angular dependence of the amount of x-ray translation.

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I. INTRODUCTION

The in-depth property of material in real space causes topological property, leading to the development of topological wave guides and laser oscillations and other topological photonics applications [1–4]. The rapid change of the complex reflectivity of microwave radiation forms a transmission boundary mode and a localization of radiation around the aperiodic layer among the periodic multilayers in the band gap due to the generated finite geometric phase [5,6]. Geometric phase is a kind of the Berry phase for layered medium. In order to apply the technique to x-ray regimes, we here dramatically scale down the thickness of the layers, μm order to $\text{\AA}$ order of the lattice constant of a synthesized diamond crystal containing stacking faults (SFs) where the number of sublayers inside the unit cells is modulated [Figs. 1(a)–1(c)]. The lattice spacing is gradually relaxed toward the periphery, converging to a perfect crystal.

The SF is the translation dislocation, which is one of the few lattice defects the image contrast of which can be simulated using the first principles in the spherical wave dynamical diffraction theory of x-rays [7]. Interference fringes are known to be generated in Laue case diffraction on a crystalline sample hosting SF due to the interbranch scattering by crossing the interface (IF), where new waves are additionally excited in the dispersion curve (DC) aside from the case of perfect crystal [8].

In this Letter, the effects of Bragg reflection on a crystal containing SFs have been examined. To understand the effects, a dynamical diffraction calculation is required that clarifies the geometrical property of the interplay between the atomic distribution in real space and the Bragg reflected x-ray wave field in the reciprocal space. The recent Berry phase theory intuitively derives the macroscopic x-ray wave packet translation at near Bragg conditions in a Newtonian mechanics manner, analogous to optical Hall effect [9,10].

II. THEORETICAL BACKGROUND

The following equation shows the theoretically derived x-ray translation in the proximity of Bragg condition that is related to the Berry curvature in phase space, the effect of the atomic displacement coupled to the x-ray dynamical diffraction [11],

$$\Delta \vec{r} = \int \vec{f}(\vec{k}) \frac{\partial [\vec{G} \cdot \vec{u}]}{\partial r_a} dr_a, \quad (1)$$

where the repeated subscripts are summed over the dimension of space and

$$\vec{f}(\vec{k}) = \pm \frac{(\vec{e}_{\vec{k}+\vec{G}} - \vec{e}_{\vec{k}})}{2[(\Delta k)^2 + \frac{1}{4}(|\vec{k}| - |\vec{k} + \vec{G}|)^2]^{\frac{3}{2}}} \cdot (\Delta k)^2 \quad (2)$$

represents a profile in momentum space. The amount of the gap is Δk in DC, corresponding to the Darwin width as shown in Fig. 1(d). Furthermore, $r_a = x, y, z$ and $\vec{G}$, $\vec{u}$, and $\vec{k}$ are reciprocal lattice vector, deformation of lattice plane, and wave vector, respectively, and $\vec{e}_{\vec{k}} = \vec{k}/|\vec{k}|$. The position of the atom is displaced from $\vec{r}$ in a perfect crystal case to $\vec{r} + \vec{u}(\vec{r})$ in a deformed crystal case [see Fig. 1(c)]. The value of the left hand of Eq. (1) becomes maximum at the Bragg condition, $|\vec{k}| = |\vec{k} + \vec{G}|$. The orientation of translation depends on the gradient of deformation and also on the double sign of $\vec{f}(\vec{k})$ in momentum space corresponding to the sign of angle from the Bragg peak, namely α and β branches [Fig. 1(d)] [11].

Importantly, x-ray wavepacket only receives the spatial shift along $\vec{G}$ [Eqs. (1) and (2)] without a change of its wave vector [9,10]. This effect was experimentally verified in a bent silicon crystal of 0.1 mm with the dramatically huge amount of translation of $\simeq 5$ mm reaching the edge of the crystal [10]. On the other hand, the nonzero Berry curvature for x-rays propagating in the proximity of SFs resulted in identifying their types as shown hereafter.

For demonstration, we choose crystalline specimens hosting IFs of either vacancy- or interstitial-type of SF upon diamond (111) lattice plane [see Figs. 1(b) and 1(c)]. In order to induce an interbranch scattering, we use a crystal surface antisymmetrically cut to IF of SF. We clarified that a lattice deformation field exists near IF in which the lattice spacing is

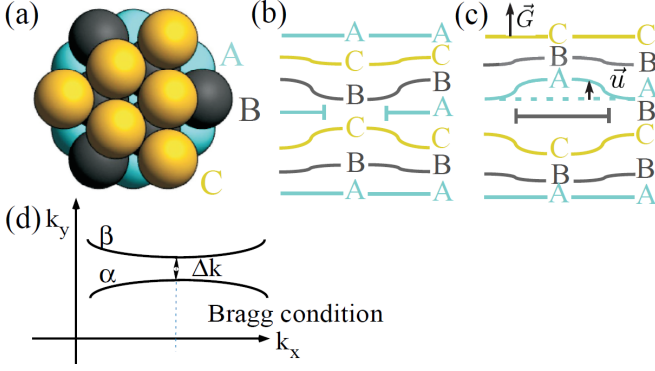


FIG. 1. (a) Schematic diagram of unit cell composed of three sublayers along diamond (111) lattice plane, named A, B, and C sublayers. The schematic diagram showing (b) vacancy-type SF with a lack of sublayer that expands lattice spacings and (c) interstitial-type SF with an additional sublayer that compresses lattice spacings. $\vec{G}$ and $\vec{u}$ represent the reciprocal lattice vector and the deformation of lattice plane, respectively. (d) Schematic DC of x-ray diffraction in a crystal, which is a crosssection for $\omega(\vec{k}) = \text{const.}$ in two-dimensional wave vector space showing the gap by Δk . α and β branches correspond to near Bragg conditions in the shallower and the deeper side of the tail of the Bragg reflection peak, respectively.

gradually relaxed, causing an x-ray translation phenomenon with its orientation reversed by the sign of gradient of deformation and the branches (α and β) of x-rays [Eq. (1) and Figs. 2(a)–2(d)]. We pay attention to the two cases where large translation occurs towards buried IF of SF from the lower part of the crystal [Figs. 2(a) and 2(d)].

As an example, we here choose a vacancy-type SF on α branch [as in Fig. 2(a)] to demonstrate this phenomenon. We assume a case where x-rays are incident on a diamond crystal, which has a surface on (100) plane antisymmetrically cut to IF of the Bragg-reflecting-(111) plane that hosts SFs [Fig. 2(e)]. DC is sketched in parallel to $\vec{G}_{111}$ shown by a purple solid line. Asymmetrically cut crystal surface functions to change the boundary condition of propagating x-rays. Excited wave is generated at intersections of DC and the green solid line, and DC and the purple solid line at area A [Fig. 2(f)] and at area B [Fig. 2(g)], respectively. Green and purple lines are in parallel to $\vec{G}_{100}$ and $\vec{G}_{111}$. Note that the wave vector components along the plane of incidence are preserved. Two waves are excited on the α and β branches at area A, denoted by a blue-filled circle ($\vec{k}_{O_1}$ on α branch) and a red-filled circle ($\vec{k}_{O_2}$ on β branch) along a line in parallel to $\vec{G}_{100}$ [Fig. 2(f)].

Two effects terminate the x-ray translation effect when x-rays reach the buried inclined IF and the upper wedge of the crystal. First, the shift is significantly reduced due to the local off-Bragg condition where $\Delta\vec{r} \simeq 0$ is realized in Eq. (1). Second, interbranch scattering [8] occurs at IF due to the change of the boundary condition, which can excite additional waves on DC. The new wave denoted by a new blue-filled circle will be generated on the α branch along a line in parallel to $\vec{G}_{111}$ [Fig. 2(g)]. Its group velocity vector shown by orange arrow in Fig. 2(g) indicates that the dominant energy flow is in a transmission direction. The unpreserved x-ray wave vector inside the crystal results in the termination of the x-ray

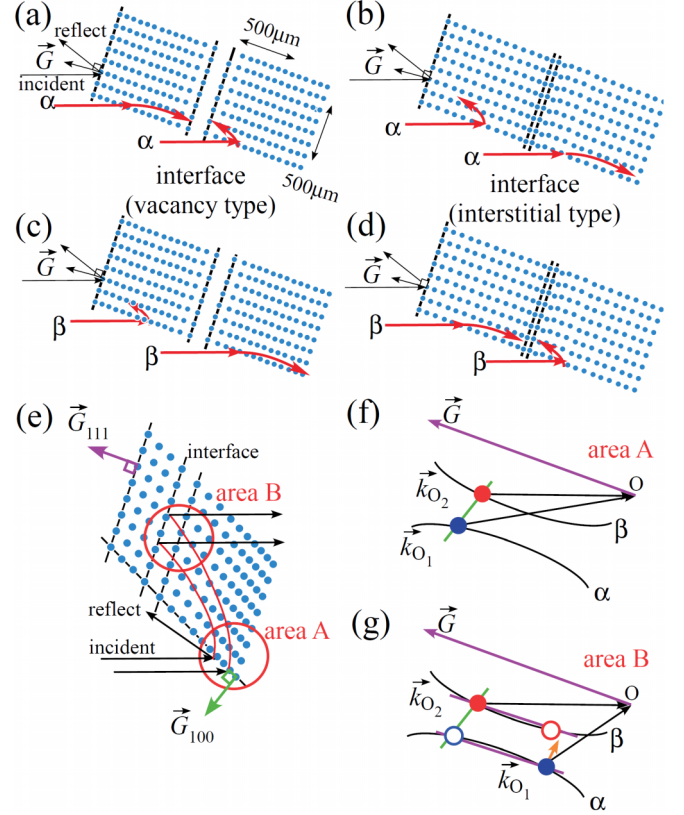


FIG. 2. Schematic diagram of x-ray translation effect when x-rays are irradiated onto a side surface of a crystal. Its orientation is reversed due to two conditions, branches [α (a), (b) and β (c), (d)] on DC and the type of SF [vacancy type (a), (c) and interstitial type (b), (d)] having the reversed sign of gradient of deformation. In Figs. 2(a) and 2(d), the x-rays incident from the left into the bottom part of the crystal are led toward IF. (e) Diagram of the phenomena around IF of SF [for Fig. 2(a)] with two deflections. (f) Schematic DC at area A. Waves denoted by blue- and red-filled circles are excited along a green line in parallel to $\vec{G}_{100}$. (g) Schematic DC at area B. An additional wave on the α branch is excited at new blue-filled circles along a purple line in parallel to $\vec{G}_{111}$ whose group velocity vector is shown by orange arrow, in direction of normal of DC. The unpreserved x-ray wave vector, indicated by the shift of blue filled circle $\vec{k}_{O_1}$ from (f) to (g), results in the termination of the x-ray translation effect. Birefringence by two waves (blue filled and open circles) forms the interference fringes inside crystal wedge downstream of IF [Fig. 2(e)].

translation effect and the x-ray trajectory is deflected at area B to propagate in the direction of the incident beam.

The interference fringes are generated by the two waves, blue filled and blue open circles [Fig. 2(g)], through the crystal wedge downstream of inclined IF of SF analogous to Pendelösung fringes [12].

III. EXPERIMENTAL SETUP

For the experiment, we selected a single diamond crystal hosting buried SFs along diamond (555) lattice plane, inclined by 54.7 degrees relative to the diamond (100) crystal surface. The high-quality diamond crystal was synthetically grown using the Czochralski method by Sumitomo Electric

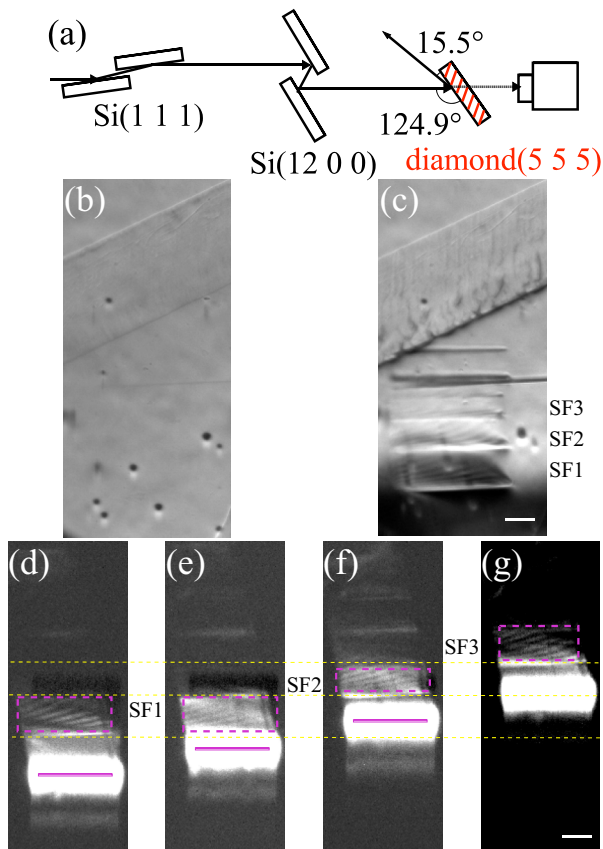


FIG. 3. (a) Experimental setup with a double crystal monochromator and a channel cut crystal in $(++)$ geometry to reduce the angular divergence of the incident beam. Whole beam transmitted image through diamond crystal (b) at off-Bragg condition and (c) at near Bragg condition of diamond (555) lattice plane hosting SFs. Prominent interference fringes at IFs of SFs (SF1-SF3) are observed in (c). (d)–(g) Transmitted image of a diamond crystal by changing the incident x-ray position on the sample, limited by incident cross slit ($10\text{ }\mu\text{m}$ vertical width, purple solid box). The x-rays are translated upwards to reach IFs of SF1-SF3 (purple dotted boxes) where interference fringes are observed. (d)–(g) The amount of the X-ray translation was on the order of $400\text{ }\mu\text{m}$ at the downstream detector plane. Scale bars are (b), (c) $200\text{ }\mu\text{m}$ and (d)–(g) $200\text{ }\mu\text{m}$ and exposure time are (b), (c) 2.5 sec and (d)–(g) 10 sec, respectively.

Corp., Japan [13]. It is a type IIa diamond which has minimal impurities and crystalline defects. The variation in the orientation of the crystal plane is smaller than $1\text{ }\mu\text{rad}$ over the entire crystal. We selected 16 keV x-rays from an undulator light source at BL29XU [14] of the SPring-8 facility with a 22.83 mm gap, which was guided to Experimental Hutch 4 (EH4). For sensitive detection of the x-ray translation effect, the angular divergence was set to be $\simeq 1.3\text{ }\mu\text{rad}$ by setting a Si(111) monochromator and a Si(1200) channel cut crystal (CCC) in a $(++)$ geometry [see Fig. 3(a)]. It is significantly narrower than the Darwin width of the diamond (555) plane of $\simeq 1.7\text{ }\mu\text{rad}$. The Bragg angle of CCC and diamond (555) plane were 58.9 and 70.2 degrees, respectively. In order to detect the transmitted image at around the area of SF, an x-ray image sensor [15] with the effective pixel size of $6.5\text{ }\mu\text{m}$ was set at around 31 and 65 cm downstream of the diamond crystal

for two different occasions of the experiments. We observed the transmitted images using both with the whole beam and with the narrow beam, limited by an incident cross slit ($10\text{ }\mu\text{m}$ vertical width and $500\text{ }\mu\text{m}$ horizontal width), in the following experiments.

IV. EXPERIMENTAL RESULT

A. Anomalous bending

The whole beam transmitted image was observed without any particular structures of SFs at off-Bragg condition [Fig. 3(b)], which exhibited prominent interference fringes in areas denoted by SF1-SF3 in the proximity of the Bragg reflection condition [Fig. 3(c)]. For detailed investigation, narrow areas were irradiated by an incident cross slit ($10\text{ }\mu\text{m}$ vertical width) and the slit position was shifted in the vertical direction around the area containing SF1-SF3 [Fig. 3(c)].

The observed transmitted x-ray image downstream of the cross slit manifested that the shift of x-rays is toward upwards. This is most likely due to the x-ray translation effect that has an order dependence of the diamond reflection plane, the amount of which is inversely correlated with the acceptance angle of crystal [Eqs. (1) and (2)]. The shift of the translated x-rays, however, is terminated at a nearly fixed height regardless of the height of the slit and does not go beyond interference fringes (purple dotted box) [Figs. 3(d) and 3(e)]. The translation effect appeared to be terminated at IF of SF1 and negligible propagation was observed above this IF.

By raising the incident position further upwards, similar interference fringes and propagation toward IF of SF2 [Fig. 3(f)] and SF3 [Fig. 3(g)] were observed. These propagations were terminated at these IFs. These results strongly support that x-ray deflection occurs twice, first by the x-ray translation toward buried IF of SF1-SF3 by the deformation nearby IFs, and second at these IFs as sketched in Fig. 2(e). Due to the unchanged wave vector during the propagation inside the crystal, the second deflection of x-rays occurs into a direction parallel to the incident x-rays at IF of SF1-SF3 due to the termination of the x-ray translation as a result of the interbranch scattering [8].

The bottom of IF appears brightest as seen especially in Figs. 3(d)–3(g) which means that the x-ray translation effect is so effective as to force the x-ray wavepacket to propagate near the crystal surface. The image contrast is enhanced to see the distribution of the translated x-rays, having the brightness of $\simeq 2\%$ of that of the transmitted x-rays through the slit.

Interference fringes analogous to Pendellösung fringes [12] are observed at a single IF of SF due to the interbranch scattering [8], which provide a direct knowledge of the surface of the buried IF of SF.

B. Anomalous transmission

Using the whole beam transmitted image, which makes the x-ray translation effect less noticeable, the angular dependence was investigated around SFs, at the bottom of IF of SF2 [inside the dark green box in Figs. 4(a)–4(d)]. Figure 4(d) showed a drop of transmissivity due to the occurrence of Bragg reflection which is approximated well by a gaussian function. It also showed a sharp rise of transmissivity in the

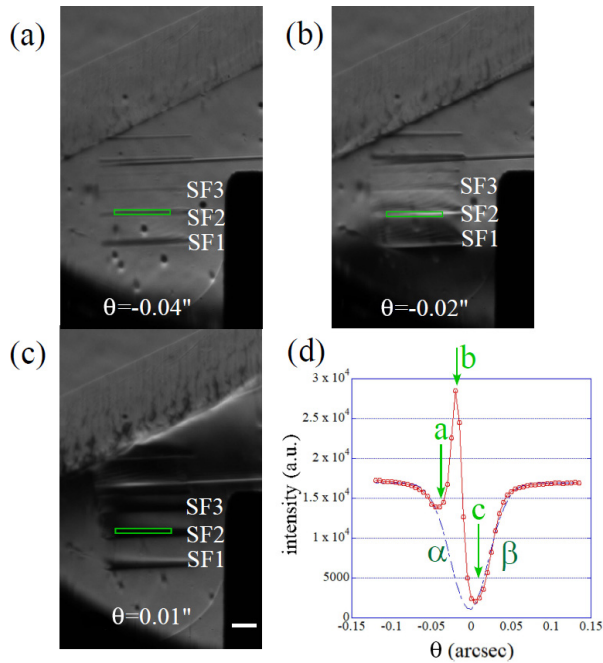


FIG. 4. (a)–(c) Angular dependence of whole beam transmitted image around SFs (SF1–SF3) with offset angle from the Bragg peak of (a) -0.04 , (b) -0.02 , and (c) $+0.01$. (d) Intensity at the bottom of IF of SF2 [within dark green boxes in Figs. 4(a)–4(c)]. A reduction of transmissivity was observed by the Bragg reflection near the Bragg angle, modeled by a blue dotted Gaussian function. A sharp transmissivity enhancement was observed in the lower angular tail (α branch) of the Bragg reflection curve at around the offset angle of Fig. 4(b). The enhanced transmissivity was observed within the band gap of the Bragg reflection. Scale bar is (a)–(c) $200\ \mu\text{m}$.

lower angular tail of the Bragg reflection curve [offset angle = -0.02° in Fig. 4(b)], in the α branch. The anomalous

transmissivity should have been caused by the aperiodic unit cells among periodic unit cells, analogous to the result using microwave radiation [5]. The enhanced transmissivity at the peak, larger than the one at off-Bragg angle, should be due to focusing toward IF by the x-ray translation and its occurrence in the α branch enables us to discriminate the stacking fault to be the “vacancy type” as shown schematically in Figs. 2(a) and 2(e).

V. CONCLUSION

To summarize, we observed an anomalous bending and transmission at the Bragg condition by crystal stacking fault. Two macroscopic and sharp deflections were observed in the proximity of the atomic interface of stacking faults inside a diamond crystal due to the x-ray translation effect. An anomalous transmissivity was observed, which is analogous to the one observed with microwave radiation around the aperiodic layer inside the periodic multilayers by generated finite geometric phase [5,6]. This was further enhanced by the x-ray focusing caused by X-ray translation toward the interface. The occurrence of the enhanced transmissivity in the α branch enabled us to discriminate the stacking fault to be the “vacancy type” by the angular dependence of the amount of x-ray translation. An x-ray crystal nanophotonics will be cultivated which makes use of the x-ray translation and the geometric phase to control the x-ray trajectory and the transmissivity, by artificially introducing a gradual and a discontinuous modulation of in-depth lattice spacing, e.g., through the monolayer-doping into crystals [16].

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