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Emitter-site specificity of hard x-ray photoelectron Kikuchi-diffraction

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Abstract

High-resolution full-field imaging of \((k_x, k_y)\) photoelectron distributions \((k\)-resolution 0.03 Å\(^{-1}\), angular resolution 0.03° at 6.7 keV\) in a large field of view (up to 16 Å\(^{-1}\) dia.) allows to observe fine details in Kikuchi-type diffractograms. Alongside with the element specificity via core-level spectra, this method opens a new avenue to structural analysis using hard x-ray photoelectron diffraction (hXPD). Here we present a theoretical study of the emitter-site specificity by simulating hXPD patterns for arbitrary positions of emitter atoms in the unit cell. Using the Bloch wave approach to photoelectron diffraction from lattice planes, the diffraction patterns from a number of positions in the unit cell can be obtained simultaneously exploiting the reciprocity theorem. Simulations for dopant atoms and dopant multimers (dimers, trimers, clusters) in the Si lattice at various positions in the unit cell reveal a strong site-sensitivity in terms of dramatic changes in the diffraction patterns with emitter-atom position. The results are compared with measurements for Si hyperdoped with Te.

1. Introduction

Owing to its element specificity, x-ray photoelectron diffraction (XPD) bears a high potential for structural analysis [1–6]. Recent work addressed the fascinating aspect that dopant atoms can be selected via their core-level photoemission signals [7, 8] and their XPD-patterns can be compared with those of the atoms in the host lattice. One of the intriguing advantages is that the method can easily be combined with electronic structure analysis using angle-resolved photoelectron spectroscopy (ARPES) in the soft- and hard-x-ray range. The latter method for bandmapping of the true bulk electronic structure finds rapidly growing interest [9–12].

The new experimental approach to ARPES and XPD employing full-field momentum imaging has proven particularly powerful for this combined analysis. In a first model study in the hard x-ray range, hard x-ray photoelectron diffraction (hXPD)-patterns have been recorded for a graphite single crystal at many photon energies [13]. The measurement yielded detailed Kikuchi-type diffraction patterns, which showed an excellent one-to-one agreement with simulations using the Bloch-wave approach [14]. The excellent agreement (including the faint fine structure in Kikuchi bands and zones) of calculated and measured hXPD patterns suggests to use this method as sensitive tool for structural analysis. The full-field imaging is highly efficient; in the case of the strong C 1s core-level signal of graphite a hXPD pattern is recorded within 10 min. The Bloch-wave simulation method is highly efficient as well, because it allows to calculate the Kikuchi patterns in terms of Bragg scattering of electrons from point sources inside a crystal using a rather
small number of Fourier components of the scattering potential (equivalent to sets of lattice planes), as described in [15–17].

Full-field imaging XPD is also important for ARPES studies at high energies, where the band patterns can be strongly modulated by XPD. In a new generation of hard-x-ray ARPES experiments, valence-band momentum patterns and core-level diffractograms are recorded at identical settings (kinetic energy, k-field of view) of the momentum microscope. Exactly identical kinetic energies are set via tuning of the photon energy. This allows for a multiplicative correction (pixel-by-pixel division) of the valence-band momentum pattern using the core-level diffractogram, thus eliminating the diffraction modulation to a large extent [18].

This progress concerning XPD experiments and theory comes along with the availability of hard-x-ray synchrotron beamlines and forthcoming x-ray free electron lasers. At the new beamline P22 of PETRA III a total energy resolution [combined resolution of the time-of-flight (ToF) analyzer and the photon bandwidth] of 62 meV at 6 keV (resolution \( \sim 10^{-3} \)) has been reached [19, 20]. At the free electron laser FLASH (DESY, Hamburg) a similar ToF momentum microscope is operated [21] and the first time-resolved XPD experiment with fs resolution at soft x-ray energies has been performed [22].

The element specificity of XPD can be exploited to determine the position of dopant atoms within the bulk of a host lattice, with a selected core-level signal serving as spectroscopic fingerprint. Previously, the same approach was used to study the structural properties of adsorbates on surfaces, [3, 23, 24]. In this article we address an issue of practical importance for the analysis of XPD patterns: the emitter-site specificity, which can be exploited for the location of dopant atoms or impurities in host materials. Information on dopant sites is of particular importance for semiconductor design because simultaneous occupation of different sites can take place, some of them counteracting the desired hole or electron doping effect [25, 26]. There is a wealth of previous studies concerning dopant sites, mostly using ion channelling [27], Rutherford backscattering [28, 29], near-edge x-ray absorption fine structure [30], infrared photoresponse [31], or diffraction of beta-rays from implanted radioactive nuclei [32, 33], indicating the importance of this task. XPD adds complementary information on the specific site within the translational-symmetric lattice that can only indirectly be deduced from the above-mentioned methods.

Here, we present calculated Kikuchi diffractograms for many positions of emitter atoms in the unit cell, i.e. substitutional sites, interstitial sites (tetrahedral and hexagonal) and fully arbitrary sites. The calculations have been performed for the example of the silicon lattice, due to its high technical relevance. For the particular case of Te dopants in Si, we compare the calculated results with first experimental data. The results open a new avenue towards a detailed structural analysis with high site-specificity. They are of general importance for many materials whose properties are tailored via doping.

2. Methods

2.1. Calculating Kikuchi diffraction patterns using the Bloch-wave approach

A detailed description of core-level XPD in the hard x-ray range by the Bloch-wave approach is given in [13, 15]. This approach is an implementation of the dynamical theory of electron diffraction [14, 16, 34, 35] for point emitters in a three-dimensional crystal. Here we extend the model towards the general case, where the core-level photoelectrons of a selected atom species (host lattice or dopant atom) are emitted from an arbitrary position within the unit cell. Detailed simulations have been performed for dopant atoms in the Si lattice on substitutional sites, interstitial sites and arbitrary sites. The Bloch wave model of high-energy electron diffraction considers the coherent scattering of an incoming plane wave beam by the crystal, which leads to a spatially modulated probability to find an electron at a specific point in the crystal unit cell. According to the reciprocity principle [36] this situation is equivalent to the time-reversed problem of calculating the intensity that is originating at a specific point in the unit cell and which is then diffracted into a plane wave that moves into a certain observation direction in vacuum.

The central task is the calculation of the overlap of the diffracted wave field—described as superposition of Bloch waves—with the point sources centered at the emitter atom positions. The Schrödinger equation in the formulation of an eigenvalue problem is solved using the Fourier coefficients \( \mathbf{V} \), which describe the periodic scattering potential. These Fourier coefficients have a concrete meaning: they are related one-to-one to sets of reflecting lattice planes, parametrized by reciprocal lattice vectors \( \mathbf{g}_{hkl} \). The corresponding lattice-plane spacings are \( d_{hkl} = 2\pi / \mathbf{g}_{hkl} \). The eigenvalue problem for a general complex matrix (with the matrix dimensions given by the number of reciprocal lattice vectors \( \mathbf{g}_{hkl} \)) is numerically simplified by introducing the forward-scattering approximation, which is valid for high final-state energies [37].

The efficiency of the Bloch-wave approach lies in the fact that the large number of scatterers within the interaction volume (\( 10^3 – 10^6 \)) is replaced by a small number of relevant reciprocal lattice vectors (i.e. sets of
lattice planes). Figure 6 in [13] demonstrates that for graphite just 25 diffracted beams (i.e. sets of lattice planes) are sufficient to describe a characteristic photon-energy dependence of the fine structure inside the central zone (crossing region of Kikuchi bands), in fair agreement with experiment.

The question arises, whether the \( k \)-space consideration forming the basis of the Bloch-wave model provides a realistic description of experimental hXPD patterns. We can clearly answer this question: the excellent one-to-one agreement in the case of graphite down to final-state energies as low as 2.6 keV clearly proves that despite the forward-scattering approximation the Bloch-wave model is a proper description of hXPD, at least for materials with low scattering factors like carbon (\( Z = 6 \)) [13] and GaAs (\( Z = 31 \) for Ga and 33 for As) [38]. For Si (\( Z = 14 \)) and Ge (\( Z = 32 \)) we can also expect excellent agreement between Bloch-wave theory and hXPD measurements.

Since only the Fourier components of the 3D-periodic potential are considered, symmetry-breaking at the surface as well as local distortions of the lattice close to the dopant atom are neglected. It is known from HAXPES studies that the relative contribution of the surface atoms to the total photoemission yield becomes negligible at hard x-ray energies [39]. Thermal broadening is accounted for by a Debye–Waller factor, which dampens the high spatial frequency components of the atomic potentials to describe an average, smeared-out scattering potential.

Stochastic scattering (thermal and defect scattering) destroys the coherence with the initial photoelectron wave. In valence-band photoemission the ratio between the direct photoemission channel and the background signal caused by \( k \)-randomizing scattering processes is governed by the Debye–Waller factor. This background becomes large at high energies in the several-keV range; quantitative examples are given in [18, 40–42]. Since it originates from quasi-elastic scattering, the background shows a characteristic energy spectrum termed matrix-element-weighted densities of states (MEWDOS). Full-field momentum imaging revealed that this MEWDOS background is not diffuse or isotropic but it carries the energy spectrum of the primary photoelectron wave and hXPD measurements.

Incoherent scattering in the final state has to be considered for the core-level hXPD diffractograms. The main contribution from inelastic scattering is given by electronic excitations (i.e. plasmons) which are not localized and thus lead to a plane-wave final state. These electrons, however, can be separated from the primary photoelectron signal due to the large energy losses involved (typical plasmon energies of the order of 10 eV). In complete analogy to the classical Kikuchi process, any secondary, localized incoherent scattering processes would show a similar pattern as it would be observed in an SEM at the same energy, which is challenging to separate from the primary photoelectron signal for quasi-elastic energy losses in the range of a few meV corresponding to localized phonon excitations. This secondary Kikuchi pattern represents an average over all scattering sites, weighted by the atom-specific scattering factors, i.e. the memory for the initial photoemitter would be lost. The total observed pattern would be the sum of the site-specific core level hXPD pattern generated through diffraction of the primary photoelectron wave and the secondary, quasi-elastic scattering-induced Kikuchi pattern (weighted by the Debye–Waller-factor). At very high energies, even cascade-like successes of such quasi-elastic events in coexistence with the coherent diffraction of the primary photoelectron wave can occur [43]. At energies of 3–6 keV we do not expect significant cascade effects, but individual quasi-elastic incoherent scattering events at impurities or due to thermal vibrations can be important. Experiments have shown, however, that even at room temperature the element specificity still persists, i.e. the contribution from localized large-angle quasi-elastic scattering events is not dominating the signal. We assign this to the increased path length of trajectories which results from such events, which will increase the probability of inelastic scattering by plasmons and other electronic excitations, which do not contribute to the diffraction signal at the energy of the primary core-level photoelectron.

### 2.2. Full-field recording of photoelectron diffractograms using hard x-rays

The calculated hXPD patterns are compared with experimental data recorded at beamline P22 [19] of Petra III at DESY (Hamburg). The experimental setup has been described in detail in [13]. A special high-energy objective lens yields a momentum image of photoelectrons with initial kinetic energies of up to >7 keV in its backfocal plane. This \( k_x-k_y \) image is focused by a zoom optics via a low-energy drift section to the image detector, in our experiment a 3D-recording delay-line detector (DLD). The DLD resolves \( k_x-k_y \) patterns via the momentum coordinates and an energy interval of several eV width via the ToF. The diffractograms are observed directly in reciprocal space (i.e. on the transversal momentum scale \( k_y \)) instead of real-space polar coordinates as in conventional XPD experiments using hemispherical analyzers. The observable \( k \)-field of view is up to \( \sim 16 \) Å\(^{-1}\) at 6.7 keV, corresponding to a small polar angular range of 0–11°. The \( k \)-resolution is \( \sim 0.03 \) Å\(^{-1}\) corresponding to an angular resolution of 0.03° at 6.7 keV. Larger off-normal observation angles are accessible by polar rotation of the sample using a mode with zero extractor field [20]. The real-space
Figure 1. Sequence of measured (a)–(e) and calculated (f)–(j) hXPD patterns of the Si 2p core level at final-state energies between 4.69 and 6.69 keV. The width of the {220}-type Kikuchi bands and central zone is given by $G_{220} = 3.27 \, \text{Å}^{-1}$. (f)–(j) Calculated Si 2p XPD-patterns; the $k$-scale is identical in all panels. Enlarged regions and arrows mark characteristic details, see text. (k) Magnified hXPD-pattern as measured (left half) and calculated (right half) for 5.19 keV; the arrows mark the {110}-type Kikuchi band, the marked square is shown with a different grey scale. (l) Measured hXPD pattern at 4.69 keV with marked Kikuchi lines and bands as well as reciprocal lattice vectors. (m) Unit cell of the Si lattice.

observation mode (PEEM mode) facilitates checking the footprint of the photon beam and the surface quality and allows an easy selection of the desired sample area. The 3D recording architecture of parallel $k$-imaging and ToF recording of the binding energy $E_B$ counteracts the intensity/resolution problem of hard-x-ray ARPES [18].

Full-field imaging offers valuable possibilities of image processing, like subtraction or division of different images, a simple way of checking for differences. In order to eliminate effects of electron optics (chromatic aberration) and to compare identical dynamical diffraction conditions it is essential to bring the signals of interest to identical kinetic energies. This is facilitated by tuning the photon energy such that the photoelectrons whose momentum patterns are to be compared have exactly the same kinetic energy. This ensures artefact-free ratio images as required for the elimination of the diffraction signature in VB-patterns [18] or for a detailed comparison of diffractograms from different atom species in order to determine lattice sites (see below).

The simulated hXPD diffractograms are compared with measurements for a Si(001) single crystal with implanted Te atoms [28]. Previous work [27] shows that the increase of Te concentration leads to changes in electronic conductivity from nearly insulating (light doping) to quasi-metallic at low temperature (doping level of our sample). The thickness of the Te-rich layer is approximately 120 nm [28, 31] i.e. much thicker than the information depth of our experiment (~20 nm). An inhomogeneous depth profile of the dopant concentration appears in the experiment as averaged signal, weighted with the attenuation factor due to the inelastic mean free path.

Prior to the measurement, the surface was etched using diluted hydrofluoric acid followed by an ethanol wash and rapid introduction into the vacuum system.

3. Results

3.1. Host lattice and substitutional sites

The emitter-site specificity of the hXPD patterns was studied by Bloch-wave calculations for various emitter-atom positions $R_{em}$ in the unit cell. The calculations relate the amplitude of the wave-field pattern at the position $R_{em}$ in the crystal with the intensity of the wave in vacuum with wave vector $k_{vac}$. Slight variations of $k_{vac}$ can cause strong changes of the amplitude at position $R_{em}$, especially for directions close to the Bragg condition. In the framework of the reciprocity theorem [44] the multiple elastic scattering in the periodic scattering potential establishes a 'bi-directional correspondence' between the wave amplitude at position $R_{em}$ in the unit cell and the far-field amplitude with wave-vector $k_{vac}$.
The expected good agreement between experiment and calculation is seen by the comparison of the measured and calculated Si 2p diffractograms for the (001)-surface, shown in figures 1(a)–(e) and (f)–(j), respectively. The final-state energy (kinetic energy of the photoelectrons inside the crystal) ranges from 4.69 keV to 6.69 keV. At these energies the diffraction patterns are dominated by the horizontal and vertical (220)-type Kikuchi bands with width given by the reciprocal lattice vector $|G_{220}|$ as marked in (a) and (f). Further Kikuchi bands and lines are denoted in (l). Detailed inspection of measured and calculated hXPD patterns reveals very good agreement throughout the entire energy range. Note the one-to-one agreement of many fine details, e.g. the doubling and the rounded corners of the squares in (d) and (i) and the narrow moon-shaped features in (e) and (j), marked by arrows. The agreement is emphasized in the magnified panel (k), where the left and right halves show the measured and calculated patterns, respectively. Except for a slightly larger blur of the experimental pattern, all details in the diffractograms agree remarkably well. This proves that for Si ($Z = 14$) the Bloch-wave approach with forward-scattering approximation constitutes an excellent model yielding almost perfect agreement.

The central zone (bright crossing region of the horizontal and vertical Kikuchi bands) is particularly sensitive to subtle details of the dynamical diffraction, as we have investigated for graphite (see, e.g., figure 6 in [13]). In figure 1(k) this bright zone shows good overall agreement as well, but in addition slight differences appear to be significant.

Please notice that the width of the Kikuchi band edges has an intrinsic limit, which is determined by the size of structure factors which enter into the dynamical theory. Thus, it is not possible to measure perfectly sharp patterns for a perfect crystal. The sharpness of the Kikuchi patterns even from a perfect crystal is limited by the atomic scattering potentials [45, 46]. As extrinsic reason the measured pattern could be blurred due to the limited $k$-resolution of the electron optics, which is given by $\sim 500$ resolved points along the image diagonal.

The calculated hXPD patterns are the sum of two patterns calculated for the sites $R_{\text{em}} = (0, 0, 0)$ and $(0.25, 0.25, 0.25)$ of the two Si atoms A and B in the unit cell, cf figure 1(m). It means that the patterns in figure 1 represent the hXPD signatures of dopant atoms on substitutional sites, for the kinetic energies as given in the panels. This energy determines the photoelectron wavelength and governs diffraction dynamics. Experimentally, the kinetic energy is adjusted by setting the proper photon energy using the monochromator.

### 3.2. Interstitial sites

Interstitial sites in the diamond and zincblende lattices can host dopant atoms and play an important role for the action of dopants. Early calculations [47, 48] for dopants in GaAs revealed that interstitial atoms can act as ‘nucleation centers’ for clusters which, in turn, can compensate or even reverse the desired donor or acceptor action of the dopant atoms. The diamond-type lattice has four types of interstitial sites: bond-center interstitial (point symmetry: $D_{3d}$), hexagonal interstitial $\text{hex} (D_{3d})$, tetrahedral interstitial ($T_d$) and split-(001) interstitial ($D_{2d}$) [49, 50]. The tetrahedral interstitial site is the energetically preferred site for dopants like, e.g. Li, whereas the hexagonal interstitial site plays a role in the diffusion of small atoms where it acts like an energetic saddle point [47].

Figure 2 shows the calculated hXPD patterns for core-level photoelectrons with a final-state energy of 5.19 keV of dopant atoms in interstitial sites within the Si lattice. Calculations were done separately for the five tetrahedral sites [examples in (a) and (b)] at $R_{\text{em}} = (0.5, 0.5, 0.5); (0.75, 0.75, 0.75); (0.25, 0.25, 0.75); (0.75, 0.25, 0.25); (0.25, 0.75, 0.25)$ as well as the four hexagonal sites $(f)$ and $(g)$ at $R_{\text{em}} = (0.375, 0.375, 0.375); (0.875, 0.625, 0.875); (0.875, 0.125, 0.375); (0.375, 0.125, 0.875)$. The positions in the unit cell are denoted in figure 2(d); for sake of clarity, the $T_d$ sites 1–5 are marked in the upper unit cells, the $\text{hex}$ sites 1–4 in the lower ones. The two hXPD-signatures of the $T_d$-sites are only two-fold symmetric. They are rotated by 90° with respect to each other. For the split-(001) structures, the interstitial atom cannot be distinguished from one of the host atoms [49]. All $\text{hex}$ interstitial sites show no rotational symmetry; the only symmetry element is a horizontal (site 2 in figure 2(g)) or vertical (site 1 in figure 2(f)) mirror plane. Since the dopant atoms would occupy energetically-identical sites statistically, the Kikuchi patterns that would be observed in an experiment are the average of all equivalent tetrahedral or hexagonal sites (see figures 2(c) and (e)).

We conclude that dopant atoms on interstitial sites have very different hXPD-signatures, most strikingly visible in the intensities in the central zone. Moreover, both are substantially different from the hXPD-signature of the substitutional-site at 5.19 keV, figures 1(b) and (g). The latter has pronounced bright spots at the four corners of the central diamond and at the outer tips of the triangles surrounding the central diamond. These bright local spots are missing in both the $T_d$- and the $\text{hex}$-interstitial hXPD signatures.
3.3. Arbitrary sites of a single emitter

Figure 3 shows a sequence of calculated hXPD patterns for core-level photoelectrons from a single dopant atom in Si at a final-state energy of 5.19 keV. The emitter position is varied along the (111)-direction (space diagonal) of the cubic unit cell (a)–(f); the coordinate given in the panels runs along the space diagonal from 0.0 to 0.25 (meaning $R_{em} = (0, 0, 0)$ to $(0.25, 0.25, 0.25)$). The diffractograms in figures 3(g)–(i) correspond to hexagonal and tetrahedral interstitial sites with coordinates of $R_{em} = (0.375, 0.125, 0.875); (0.25, 0.75, 0.25)$ and $(0.75, 0.25, 0.25)$.

The sequence reveals how strongly the hXPD diffractogram varies when shifting the dopant atom along the diagonal (a)–(f). Patterns (a) and (f) at 0.0 and 0.25 represent the substitutional sites, i.e. the basis of the non-primitive Si unit cell. The two patterns show only a twofold symmetry and differ in detail by a 90°
rotation, reflecting the different local arrangement of the sites A and B. The patterns figures 2(a) and (b) and figures 3(h) and (i) show the signatures of the four tetrahedral interstitial sites. There are five non-equivalent interstitials in the unit cell, whose Kikuchi patterns differ by a $90^\circ$ rotation.

Like in a conventional diffraction experiment it is not possible to derive the real-space pattern from a diffractogram, because the phase information is lost. Rather, the approach for an analysis of coexisting sites is as follows: the simulated patterns for the different sites are added with tentative weighting factors (different sites add up coherently). The sum pattern is then compared with the measured pattern. By varying the weighting factors one can get an estimation for the relative contributions of different sites. This 'best fit ratio' can be quantified using the normalized cross correlation coefficient (NCC). This was demonstrated for polarity determination and phase determination of Kikuchi patterns in [51]. The use of the NCC for quantitative pattern comparison can be envisioned in future applications of hXPD, similar to the use of an $R$-factor [52].

For an unambiguous determination of a certain site it is advantageous first to search for a characteristic detail feature by calculations and then look for this detail feature in the experiment. The search for such features could also include emission angles far away from normal emission, because the objective lens can be operated in a field-free mode, allowing for a strong tilt of the sample [20].

In fact this field-free mode is of importance not only for recording large off-normal angles of planar samples but also for future studies on small crystallites or other 3D-structured samples or corrugated surfaces. 3D corrugations lead to local distortions of the extractor field, which, in turn, deflect the electron trajectories and distort the hXPD images. A simple way to eliminate such distortions is to work without extractor field. The common understanding is that the extractor field is required in order to reach a high resolution. However, this argument is not valid in the regime of high kinetic energies (several keV) and small footprints of the photon beam on the sample. An example is shown in figure S1 (https://stacks.iop.org/NJP/22/103002/mmedia) in the supplement, where we compare ray tracing calculations with and without extractor field for a kinetic energy of 6 keV. The imaging quality is very similar. However, in the zero field mode the collecting effect of the extractor field is missing and hence the recorded $k$-field-of-view is smaller. The existence of a strong electric field at the sample surface is prohibitive for certain types of samples. Since it strongly increases the possibilities of full-field hXPD measurements, the 'zero-field mode' will be frequently used in future studies.

Another way to emphasize certain details is the choice of the proper final-state energy. This dependence is illustrated by the two series in figure S2 for $E_{\text{final}} = 5.19$ (a)–(f) and 6.19 keV (g)–(l). The filigree fine structure inside of the bands and in particular in the central zone changes substantially, compare the magnified details of the central zone. The central zone of the $\{220\}$ Kikuchi band reverses contrast from bright to dark with the shift of the emitter atom along the space diagonal.

Close inspection of the details of hXPD patterns reveals that significant differences are visible even for small shifts of the emitter position ($\sim$0.15 Å). We did not study this sensitivity in detail but will discuss this point in the context of possible dimers or clusters in the next section.

3.4. More than one dopant atom in the unit cell, dimers, trimers and clusters

Owing to its reciprocity ansatz, the Bloch-wave approach is capable of calculating the diffraction patterns of an arbitrary number of emitters in the unit cell simultaneously. Hence, it is straightforward to calculate the hXPD patterns of dopant dimers, trimers or clusters without additional computational effort. During the calculation process, the diffractograms of the chosen number of emitter positions inside the unit cell are averaged.

At a given final-state energy, hXPD patterns are not sensitive to the type of emitter atom (except for the binding energy of the core levels, which is accounted for by the photon energy). We have seen, however, that the patterns react strongly upon changes in their position in the unit cell. In addition, there are two effects, which need to be considered. First, due to the size of the dopant atoms or as result of a charge transfer, the nearest neighbour atoms of the host lattice might change their position, i.e. a relaxation of the immediate vicinity of the emitter atom can take place. Since the hXPD patterns bring out the long range order of the lattice, such a local distortion is to first order invisible in the diffractograms. Second, the dopant atoms themselves could be shifted out of a substitutional or interstitial position due to interaction with their neighbours, e.g. due to dimer bond formation. It is clear from figures 3 and S2 that this kind of relaxation acts on the diffractograms.

Figure 4 quantifies this effect of relaxation out of the substitutional sites upon dimer formation, with the interatomic axis oriented along the $\langle 111 \rangle$-direction. We assumed four cases, a non-relaxed dimer with both atoms on substitutional sites (figure 4(a)), dimers with one of the two dopant atoms being shifted out of the substitutional position (b) and (c), and a dimer with both atoms being shifted by the same amount. We
Figure 4. Calculated photoelectron Kikuchi-patterns for a dimer of dopant atoms with axis oriented along the \langle 111 \rangle -direction on substitutional sites and at relaxed positions. (a) Both emitter atoms on substitutional sites at coordinates A (0, 0, 0) and B (0.25, 0.25, 0.25). (b) First emitter at position A', moved by 0.46 Å away from atom B. (c) Second emitter at position B', moved by 0.46 Å away from atom A. (d) Both emitter atoms A' and B' moved away from each other by 0.46 Å.

Figure 5. Calculation for two different trimers and a cluster configuration. (a)–(c) Linear trimer with three separate equal emitters along \langle 111 \rangle in the unit cell of silicon at \( R_{em} = (0, 0, 0); (0.25, 0.25, 0.25); (0.875, 0.875, 0.875); \) (d) corresponding sum pattern. (e) Equilateral triangular trimer with emitter atoms occupying three sites of a coordination tetrahedron. (f) Cluster of seven emitter atoms centered to the Si unit cell, assuming a bond length of the cluster atoms of 2.81 Å (being the bond length in Te bulk material). (g)–(i) Like the top row, but emitter positions averaged over all four equivalent \langle 111 \rangle -directions (four diagonals of the cubic unit cell). All calculations were done for \( E_{\text{final}} = 5.69 \) keV.

assumed a shift (increase of the dimer bond length) of 0.46 Å, a value that has been estimated in [28] as possible relaxation along the \langle 111 \rangle direction during dimer formation of Te atoms in the Si lattice. The calculation reveals that the relaxation of the dimer changes the diffraction patterns drastically. The pattern for the substitutional case figure 4(a) is the sum of patterns figures 3(a) and (f). If one of the atoms is shifted, figures 4(b) or (c), the fine structure has already changed significantly and if both atoms are shifted (d) the pattern looks entirely different. Only the vertical \{220\} Kikuchi band is still visible in (d), the horizontal one and the \{100\} bands in diagonal orientation are strongly masked by a puzzling system of many lines. It is clear, however, that all lines and Kikuchi bands represent the metric of \( k \)-space.

Figure 5 shows analogous results calculated for a linear trimer, an equilateral triangular trimer and a cluster of seven atoms. Since in reality the multimers would be oriented statistically along the four \langle 111 \rangle -directions, the second row shows the patterns averaged for the four directions. The linear trimer is oriented along \langle 111 \rangle, individual patterns are shown in (a)–(c), the sum pattern in (d). It is clearly seen that in the sum pattern (d) the horizontal Kikuchi band practically disappeared.

The averaging for the \langle 111 \rangle -directions can lead to disappearing of specific Kikuchi bands. For example in figures 5(i) and (l) the \{220\}-bands are absent and bands which correspond to \( G_{400} \) exhibit a strongly enhanced contrast. In the triangular configuration (figure 5(e)) three atoms occupy sites of a coordination tetrahedron: \( R_{em} = (0, 0, 0); (0.5, 0.5, 0) \) and \((0, 0.5, 0.5)\). Here the averaging for all equivalent directions yields practically the same diffraction image (k).

To perform model calculations for the cluster configuration, a \( 3 \times 3 \) Si-supercell was created and seven emitter atoms were introduced into it within octahedral configuration with the central atom at \( R_{em} = (0.5, 0.5, 0.5) \). The cluster is centered to the Si unit cell and the cluster bond length is 2.81 Å (identical to the bond length in Te bulk), which is larger than the Si–Si bond. The cluster is orientationally aligned with the
Figure 6. Measured Te 3d hXPD diffractogram of Si(001) hyperdoped with 5.6% Te [(a), from reference [53]] in comparison with Kikuchi patterns calculated for substitutional sites (b), for Te statistically-distributed on tetrahedral (c) and hexagonal interstitial sites (d). The central zone in (a) and (b) is shown with different contrast in order to avoid saturation. The final-state energy is 5.69 keV.

3.5. Comparison with experimental hXPD patterns for Te dopant in a Si crystal

Systematic calculations of different configurations in comparison with experiment can be used as a powerful new tool for a detailed analysis of the site-distribution of dopants and impurities. This approach has been used for the case of Te atoms in a Si crystal [53]. At a nominal Te content of 3 at% we can clearly observe the Te 3d core level and measure its photoelectron diffraction pattern. We notice that the effective dopant concentration in the probe volume (top 20 nm of the sample) could deviate from the nominal (average) Te abundance due to an anisotropy in the ion implantation process as well as in the solidification following the pulsed laser annealing [28].

In order to determine the prevailing sites, systematic calculations were carried out for different configurations. Figure 6 demonstrates how this method works in practice. As an example, a measured Te 3d diffractogram for a sample with 5.6 at% Te is shown in comparison with various calculations (all at $E_{\text{final}} = 5.69$ keV). The experimental Kikuchi pattern of the dopant (a) shows excellent agreement with the calculated pattern (b) for individual Te-monomers in substitutional sites (statistical sum of sites A and B). The calculations for the tetrahedral (c) and hexagonal (d) interstitial sites predict markedly different Kikuchi patterns. Hence, these sites can be ruled out as explanation for this experimental pattern (for further details, see [53]). Similarly, the seven-atom Te cluster with Te-bulk bond length, centered to the Si unit cell, shows an entirely different hXPD fingerprint (figure 5(l)).

In this case, the calculations have been performed a posteriori, hence there was no pre-selection of 'best' conditions in parameter space (final-state energy and angular range). Ideally, the calculations should be done a priori, so that the expected signature is most pronounced; see example of two final-state energies in figure S2. The present survey calculations help to find such optima for the case of the Si host lattice. For other lattices new calculations are required. On the experimental side, only a limited amount of data exists by now and mostly for undoped crystals. Moreover, measurements under large off-normal angles are very sparse. The first results (e.g. figure 2(c) in [20]) clearly show, however, that the mode without extractor field works perfectly well at kinetic energies in the several-keV range.

3.6. Relation of Kikuchi patterns and real-space probability distributions

The hXPD patterns are governed by the Fourier components of the 3D-periodic potential, i.e. the long-range periodicity. The key for understanding of the filigree fine structure lies in the point-like emitter
Figure 7. Schematic illustration of the real-space probability distribution of Bloch waves (periodic stripes) with respect to the emitter atoms related to certain details in the Kikuchi band patterns. (a) and (b) Lattice planes which form the central [100]- and [110]-type Kikuchi bands; (c)–(f) calculated diffraction patterns for different emitter atoms with positions along the ⟨111⟩-direction; (g)–(o) probability distributions of the Bloch wavefunctions in real space at selected directions (marked with different colored frames).

and the short wavelength of the photoelectrons (0.17 Å for a final state energy of 5.19 keV). A small shift of the emitter atom thus changes the phase of the Bloch-wave field and in turn the diffractogram.

To explain the qualitatively different contrast of Kikuchi bands it is easy to imagine that the probability of inelastic scattering depends on whether the electron wave field has the maximum amplitude between or at the atomic positions [16, 54]. At high electron energies, the crystal can be considered as an interferometric beam splitter that distributes electrons in a well-defined way either between or onto the atomic planes. Near the Bragg reflection, towards the middle of the band (i.e. the angles are smaller than the Bragg angle), the probability amplitude of the outgoing electrons has maxima at the atomic planes. This corresponds to the type I Bloch waves. The electrons inside this wave field will be more strongly affected by the impact of localized inelastic processes, for example phonon losses or core excitations.

Figure 7 illustrates the relation between the probability distribution of the Bloch-wave field in the atomic lattice with certain features in the Kikuchi patterns. In case of angles larger than the Bragg angle, the electron wave has maximum between the atomic planes (type II Bloch waves). Electrons moving in this type of field can escape from the crystal with significantly less inelastic collisions. Thus, to analyse the intensity in the middle of the bands (first type of Bloch waves), one needs to consider the crystal lattice structure in those directions (see figures 7(a) and (b)). The contrast of the Kikuchi band for [100] is switching from bright to dark and again to bright with emitter position changing from $R_{em} = (0, 0, 0)$ to $R_{em} = (0.5, 0.5, 0.5)$ along the ⟨111⟩-direction (see figures 7(h)). There will be high intensity in the center of the corresponding Kikuchi band where diffraction probability density overlaps strongly with those places the photoelectrons are created at (atomic positions) [15] (figures 7(c) and (g) and (f) and (j)). When the emitter atom is moved away from this position (figure 7(h)) towards the spacing between atomic planes the intensity is changing gradually (figure 7(d) arrows 3 and 4).

If the emitter atom occupies a place exactly between atomic planes (figure 7(i)) at the point with coordinates $R_{em} = (0.125, 0.125, 0.125)$, the Kikuchi band (100) shows the lowest intensity (figure 7(e)). In case emitter atom is moved to the position at $R_{em} = (0.5, 0.5, 0.5)$ it again occupies a position exactly at the atomic plane, where inelastic electrons are created and a bright Kikuchi band appears. The explanation of the intensity for the horizontal Kikuchi band (110) is the same. When the position of the emitter atom coincides with the atomic planes (figures 7(k) and (n)) the intensity is higher in contrast to the position between atomic planes (figures 7(e) and (m)). An intermediate position shows up markedly in the intensity of the rims of the Kikuchi band (figures 7(d) and (l), arrows 1 and 2). In this way, each feature in the Kikuchi pattern, seen in the far-field limit of the outgoing electron wave, can be related to a certain characteristic pattern of the probability amplitude of the Bloch-wave field in the crystal.
4. Summary and conclusions

This paper presents the theoretical proof of concept and first implementation of hard x-ray photoelectron Kikuchi-diffraction for emitter-site specific structural analysis. Using the Bloch wave approach to photoelectron diffraction from lattice planes, hXPD patterns of dopant atoms in a host lattice are simulated. The atoms of interest are addressed by their core-level signals. Chemical shifts of core-level signals due to different local configurations in the host lattice can be exploited in order to disentangle different coexisting dopant sites. Thanks to the reciprocity theorem, hXPD patterns for arbitrary positions and numbers of emitter atoms in the unit cell are calculated simultaneously, making theoretical hXPD analysis a very fast method. This property of the Bloch-wave approach gives a natural access to fully arbitrary, substitutional and interstitial sites, dimers (with and without relaxation), trimers and small clusters (with different number of emitter atoms), without much additional computational effort. All of these sites show very different hXPD signatures. In the calculations, the structures can be determined successfully with the exception of the case when the dopant material has about the same atomic number as the host material and takes exactly substitutional sites without any distortions of the host lattice. However, even in that case the experiment still allows a clear distinction of the core levels. In view of its technical importance, we have chosen silicon as host material and performed systematic calculations for various positions that are discussed as possible dopant sites. Varying the positions of dopant atoms in the Si unit cell reveals strong site-specificity of the calculated diffraction patterns. The survey study started with substitutional sites, demonstrating the difference in the non-equivalent A and B sites of the non-primitive basis of the diamond lattice. We find excellent agreement with hXPD measurements for the Si 2p core-level, proving that the Bloch-wave approach (with forward-scattering approximation) is perfect for a quantitative description of Kikuchi diffraction in this material at final-state energies of 5–6 keV. Interstitial sites (tetrahedral and hexagonal and fully arbitrary sites show very different hXPD signatures.

In the present paper, we have considered only single individual emitter sites and their effect on the hXPD zone axis fine structure. It has been shown with help of photoelectron holography using kinetic electron energies below 1 keV that the possibility of clustering of multiple dopant atoms needs to be taken into account [25] the same way as inelastic scattering and thermal vibration effects [35]. The calculation method presented here can be easily extended for such cases, and the differences between the photoelectron emission from these multiple emitters relative to single emitters with a fluctuating emission site can be sensed via the hXPD fine structure as a sensitive fingerprint in hard X-ray photoemission. Comparison of the predicted hXPD signatures with experimental results constitutes a new tool for detailed analysis of the site-distribution of dopants and impurities. As an example we show the comparison of a sequence of calculated Kikuchi diffractograms for various configurations of Te-atoms in the Si unit cell with a measured Te 3d hXPD pattern (from [53]). The core-level selective approach of full-field hXPD imaging is of general importance for a variety of materials whose properties are tailored via doping.

The results have implications for bulk-bandmapping experiments using soft or hard x-rays. The high-energy ToF microscope allows to record valence-band and core-levels patterns at identical settings and to track one-to-one changes in the geometric and electronic structures, measured quasi simultaneously. A survey study in a large range of energies revealed the presence of strong XPD signatures in the valence band patterns as well [56]. The presence of XPD-signatures in valence-band photoemission alongside with the strong emitter-site specificity found in the present work offers a fascinating possibility for future experiments. Valence-band features can be correlated with site-specific XPD signatures, revealing which atoms in a compound contribute to specific band features. To our knowledge, this information is not directly accessible by other experimental methods. Last not least, bulk sensitive momentum microscopy (band mapping combined with hXPD) opens the way to investigate temperature-dependent phase transitions in crystals, possibly with time-resolution in pump-probe experiments [21, 22, 57].

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